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# A CONTROLLED—ENVIRONMENT CHAMBER FOR ATMOSPHERIC CHEMISTRY STUDIES USING FT-IR SPECTROSCOPY

D.A. STONE

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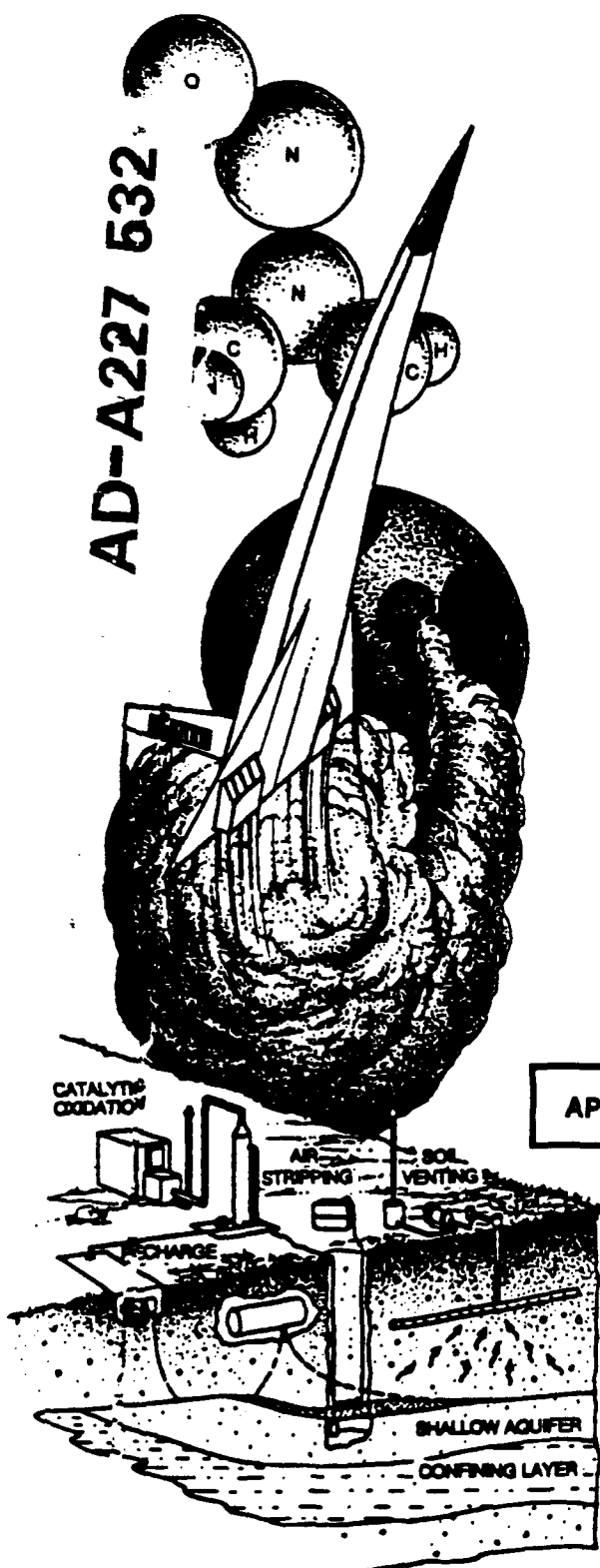
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## EXECUTIVE SUMMARY

A. OBJECTIVE: Design and construct a chamber in which to conduct fundamental studies of the atmospheric chemistry of Air Force fuels or chemicals. The chamber was to be evacuable, temperature controlled, have a minimum surface-to-volume ratio and be coated with Teflon® on the inside. It was also to contain integral long-path infrared optics so that low concentrations (0.1 - 100 parts-per-million) of reacting species could be observed and measured. It was also to have an access port through which test surfaces could be placed into the chamber.

B. BACKGROUND: Previous studies of the atmospheric fate and reactions of hydrazines were conducted in a Teflon®-film chamber. This chamber proved difficult to use because the hydrazine would simply diffuse out of the chamber through the walls. There was also no control over temperature and no way to evacuate the chamber.

C. SCOPE: The report includes chamber design goals, details of its construction, and descriptions of supporting instruments and apparatus. Typical chamber performance characteristics are described. The behavior of an inert gas (methane) and a reactive gas (hydrazine) in the chamber are described. Finally, data acquisition computer software is detailed in the appendixes.

D. METHODOLOGY: The performance characteristics of the chamber were determined by operating it under a variety of conditions designed to see if design goals had been achieved.

E. TEST DESCRIPTION: The testing was done in several parts. The ultimate vacuum capability of the chamber was determined by operating the turbomolecular pump with a full liquid nitrogen foretrap overnight. The temperature change rate and stability were determined by following changes in temperature with time at different settings on the heating/cooling recirculator. Finally, chemical stability was determined by introducing known concentrations of an inert gas (methane) and a reactive gas (hydrazine) into the chamber in dry helium and then

following their concentrations as a function of time.

F. RESULTS: A spherical design was chosen which gave the smallest surface-to-volume ratio. The chamber is a stainless steel sphere, one meter in diameter with a Teflon®-coated interior. Temperature stability is +/- 1 °C from 6.4 °C to 46.6 °C. It takes about 4 hours to go from one extreme to the other. An ultimate vacuum of  $5 \times 10^{-6}$  torr is attainable. The chamber leak rate is about 40 millitorr per day.

G. CONCLUSIONS: The controlled-environment chamber described in this report provides a valuable new platform for the characterization of vapor-phase reactions of toxic chemicals. It enables the effects of temperature, pressure, humidity, and exposure to foreign surfaces to be recorded as a function of time. This will allow researchers to collect fundamental information on chemical reactions which will aid in the prediction of the environmental fate of such chemicals.

H. RECOMMENDATIONS: Continue to enhance the operating capabilities of the chamber by improving the stability of internal optics and by adding a residual gas analysis system. In addition, explore the possibilities of conducting photochemical reactions by adding a suitable light source.

## PREFACE

This report was prepared by the Engineering and Services Laboratory, Air Force Engineering and Services Center (AFESC), Tyndall Air Force Base FL 32403-6001. Dr Daniel A. Stone (AFESC/RDVS) was the government project officer. This report summarizes work accomplished between January 1986 and June 1988, under program element 61101F.

This report has been reviewed by the Public Affairs Office (PA) and is releasable to the National Technical Information Service (NTIS). At NTIS, it will be available to the general public, including foreign nationals.

This technical report has been reviewed and is approved for publication.

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## SECTION I

### INTRODUCTION

#### A. OBJECTIVE

The research described in this report was undertaken to develop and characterize a new laboratory chamber to investigate the atmospheric chemistry of Air Force fuels and chemicals. The chamber was designed to provide control over temperature, pressure, and composition so that a wide range of experimental conditions could be prepared and maintained. It was also designed to contain a long-path optical system and to interface with an existing Fourier transform infrared (FT-IR) spectrometer so that chemical species could be identified and monitored at low (i.e., parts-per-million) concentrations.

#### B. BACKGROUND

Environmental chambers of various designs have been employed for atmospheric chemistry studies for many years (Reference 1). In our laboratory, we have conducted a number of studies on the stability of hydrazine fuels in air using a range of chambers. These have included small glass bulbs (Reference 2), large glass flasks and pipe (References 2-4), and fluorocarbon film chambers (Reference 5). These studies showed that hydrazine stability in air is a strong function of surface composition and surface-to-volume (S/V) ratio, thus the chambers themselves often controlled the decay processes. In addition, hydrazine diffusion through the walls of the Teflon® film chambers was apparently a major loss process. These earlier chambers were not temperature-controlled and the fluorocarbon-film chambers could not be evacuated.

#### C. SCOPE

This report includes chamber design goals, the details of its construction, and descriptions of supporting instruments and apparatus.

Typical chamber performance characteristics are described. Finally, the behavior of hydrazine vapor in the chamber is reported as an example of a chemical which has been studied.

## SECTION II

### EXPERIMENTAL PROCEDURES

#### A. DESIGN CONSIDERATIONS

Although a small S/V ratio is desired to minimize surface effects, there are practical limitations on the size of such a chamber. Consideration was given to the amount of gas necessary to fill the chamber, the time necessary to fill the chamber, the time necessary to pump down the chamber, and the physical size of the chamber. Geometric considerations summarized in Table 1 led to the decision to use a spherical design. The example cited in the table provides a 15 percent S/V ratio advantage over a cylindrical design and a 24 percent S/V ratio advantage over a cubic design.

TABLE 1. S/V RATIO COMPARISONS FOR VARIOUS CHAMBER GEOMETRIES FOR A VOLUME OF 1000 LITERS.

Shape	Volume (m <sup>3</sup> )	Surface Area (m <sup>2</sup> )	S/V Ratio (m <sup>-1</sup> )	$\frac{S/V \text{ (other)}}{S/V \text{ (sphere)}}$
sphere	1.000	4.836	4.836	1.000
cylinder	1.000	5.571 (R=.5 meter)	5.571	1.152
cube	1.000	6.000	6.000	1.241

Having decided on a sphere as the most effective geometry, it remained to determine a reasonable volume and size. The size difference between a 1,000-liter chamber (diameter = 1.24 meter) and a 500-liter chamber (diameter = .99 meter) was not an overriding consideration. However, the total volume was important in considering how long it would take to fill or evacuate the chamber, and the amount of gas it would take to fill the chamber (particularly in the case where compressed gas cylinders are used). In addition, the potential total path length for internal infrared optics was considered. In this regard, the 1,000-

liter chamber only offered a 25 percent increase in path length over the 500-liter chamber.

The most reasonable compromise was a chamber with a diameter of 1.00 meter. This gave a nominal volume of 500 liters, a S/V ratio of  $6.000 \text{ meters}^{-1}$ , and a practical working optical path length of 100 meters.

The chamber design required mounting/access ports on opposite sides (along the horizontal diameter line) for the long-path optics, a port (perpendicular, but in the same horizontal plane) for placing surface samples inside the chamber, view ports above each optical port for mirror alignment, and smaller ports for pumping, mixing, pressure/temperature/humidity measurement probes, and sample inlet.

Temperature control would be achieved by surrounding the chamber with copper coils attached to a recirculating heater/cooler.

## B. CONSTRUCTION DETAILS

### 1. Construction Hardware

The chamber consists of two 3/16-inch 304 stainless steel hemispheres welded together. Three 12-inch diameter by 6-inch long by 3/16-inch thick 304 stainless steel stub ends (All-Stainless, Inc.) are welded to openings in the chamber, two for optics mounting and one for sample handling. Inside the stub ends used for optics mounts, a 1/8-inch stainless steel plate is welded as a stationary platform on which mirror mounts are secured.

Above each optics port, 4-inch diameter by 6-inch long by 3/16-inch thick stainless steel pipe sections are welded to openings in the chamber to serve as view ports for optical alignment. A 6-inch stainless steel "Del Seal" flange (MDC Vacuum Products Corp., P/N F600400) is welded to each of the 4-inch pipe sections.

Three 2-inch ISO Klein Flansch (KF) half nipples (MDC Vacuum Products Corp., P/N K200-1) are welded to openings in the sphere. One for the vacuum pumping system and two for connection to pressure measurement devices.

Five 1/2-inch NPT stainless steel welding spuds (All-Stainless, Inc.) with NPT female pipe threads are welded to openings in the chamber. One for a gas inlet, one for a temperature probe, one for a humidity probe, one for a pressure transducer, and one for a drain.

The mount for a vacuum feed through mixing fan shaft is composed of a 2-3/4-inch "Del-Seal" flange assembly (MDC Vacuum Products Corp., P/N F275150) which is welded to an opening in the chamber.

Four steel tube sections, 1/2-inch ID by 2-inch long are welded to the chamber to serve as mounts for an external gas handling system. Four 2- by 2-inch angle iron legs are welded to the sphere. Four 2- by 2-inch angle iron cross members are welded to the legs to support them. The leg structure is bolted to four adjustable-height support pads.

Finally, 1/2-inch copper cooling/heating coils are welded to the chamber. A total of about 20 turns around the chamber are used.

All interior surfaces of sphere are coated with 10-20 mil FEP Teflon® (Thermtech Engineering Corp., Anaheim, CA). In addition, the mirror mounts and the inside surface of the three aluminum end caps for the 12-inch openings are Teflon® coated.

The chamber is shown schematically in Figures 1 and 2.

The view port covers are 7056 glass in Kovar® sleeves mounted in stainless steel flanges (MDC Vacuum Products Corp., P/N VP-400). They are bolted to the 6-inch "Del-Seal" flanges with O-ring seals.

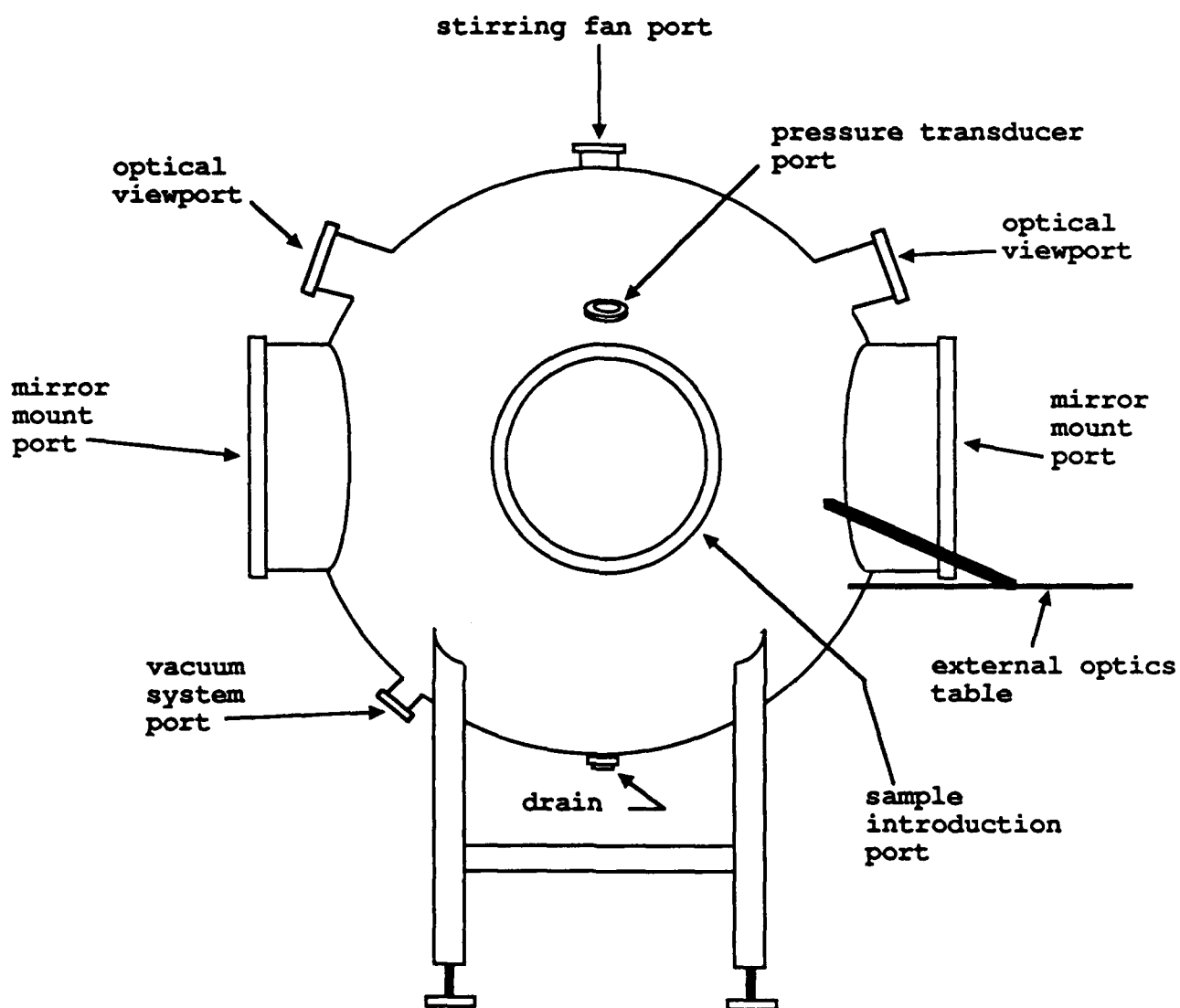


Figure 1. Schematic Diagram of the Controlled-Environment Chamber Viewed from the Sample Introduction Port Side

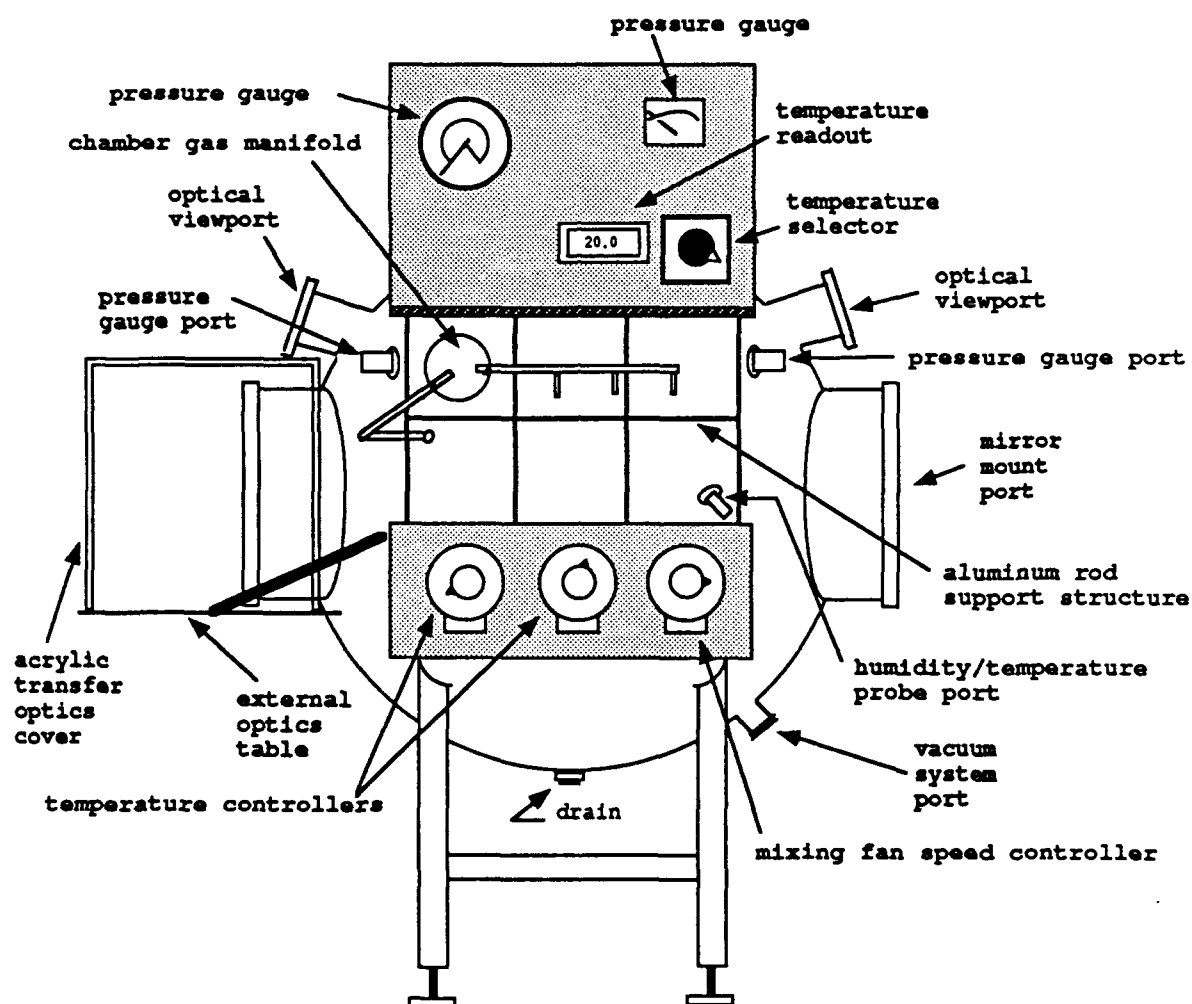


Figure 2. Schematic Diagram of the Controlled-Environment Chamber Viewed from the Side Opposite the Sample Introduction Port



The mixing fan with four 4-inch Teflon®-coated blades is coupled to an external motor (Universal Electric Co., Model AA2H136) through a vacuum feedthrough (Ferrofluidics Corp., P/N 50B103532). The feedthrough assembly is bolted to the 2-3/4-inch "Del-Seal" flange with an O-ring seal. The speed of the motor is controlled by operating it with a variable transformer set at 75 percent of full power. Power to the variable transformer is controlled by a programmable timer (Lindburg Enterprises, Inc., Chronrol CD). It is turned on continuously for sample introduction, and programmed to turn on for 3 minutes every 30 minutes during experimental runs.

The sample port cover is a 15-inch diameter plate fabricated from 1/2-inch aluminum with a 1/4-inch threaded outlet hole used for a temperature probe. It is bolted to the 12 by 6-inch stub end with an O-ring seal.

The two optical port covers are also 15-inch diameter plates fabricated from 1/2-inch aluminum. At the out-of-focus end, the cover has an additional 3-inch diameter by 3-inch long aluminum stub end attached with a bolted-on O-ring seal. This facilitated the mounting of a small, double universal joint with an exterior wall O-ring seal for path length adjustments from outside the chamber. The other three mirror mount adjustments are accessed by bored-through, 1/4-inch stainless steel male pipe O-ring compression fitting (Cajon, Ultra-Torr®) connectors which provide a seal around 1/4-inch stainless steel rods with flattened ends. These rods can be turned from the outside to adjust the mirror positions while maintaining a vacuum in the chamber. The cover is bolted to the 12- by 6-inch stub end with an O-ring seal. This optical port cover is shown schematically in Figure 3.

At the in-focus end, the port cover has two 1-3/4-inch holes to serve as entrance and exit openings for the infrared beam. A zinc selenide window (2 mm by 50 mm) is mounted over each hole with an O-ring seal. The windows are mounted above and below the horizontal center line of the port cover to conform with the overall optical path of the infrared beam as shown in Figure 4. The cover is bolted to the 12- by 6-inch stub end with an O-ring seal.

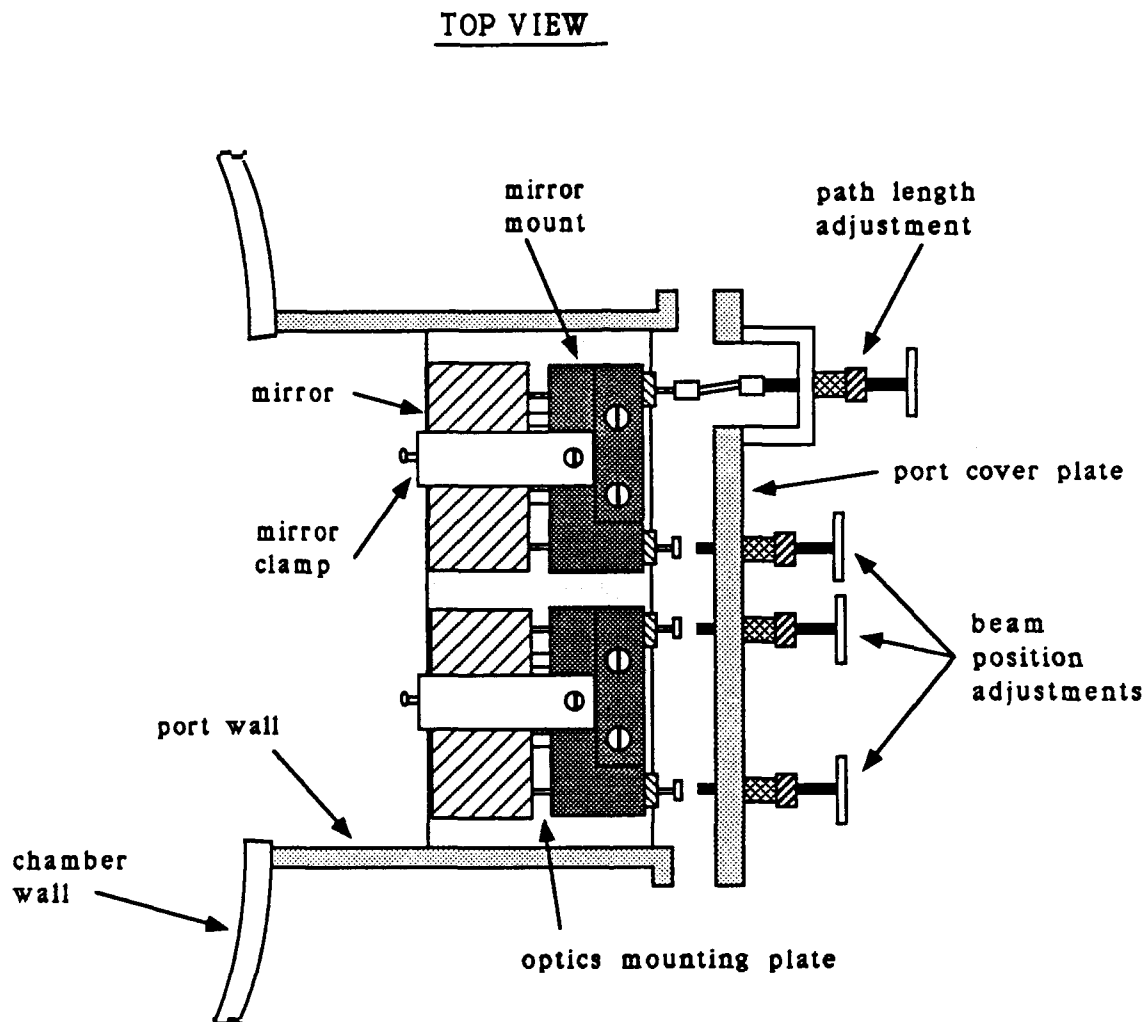


Figure 3. Schematic Diagram of the Optical Assembly Including the Two Spherical Field Mirrors (at the Out-of-Focus Location), Their Mounts, and the Port Cover Plate with Beam Position Adjustment Devices

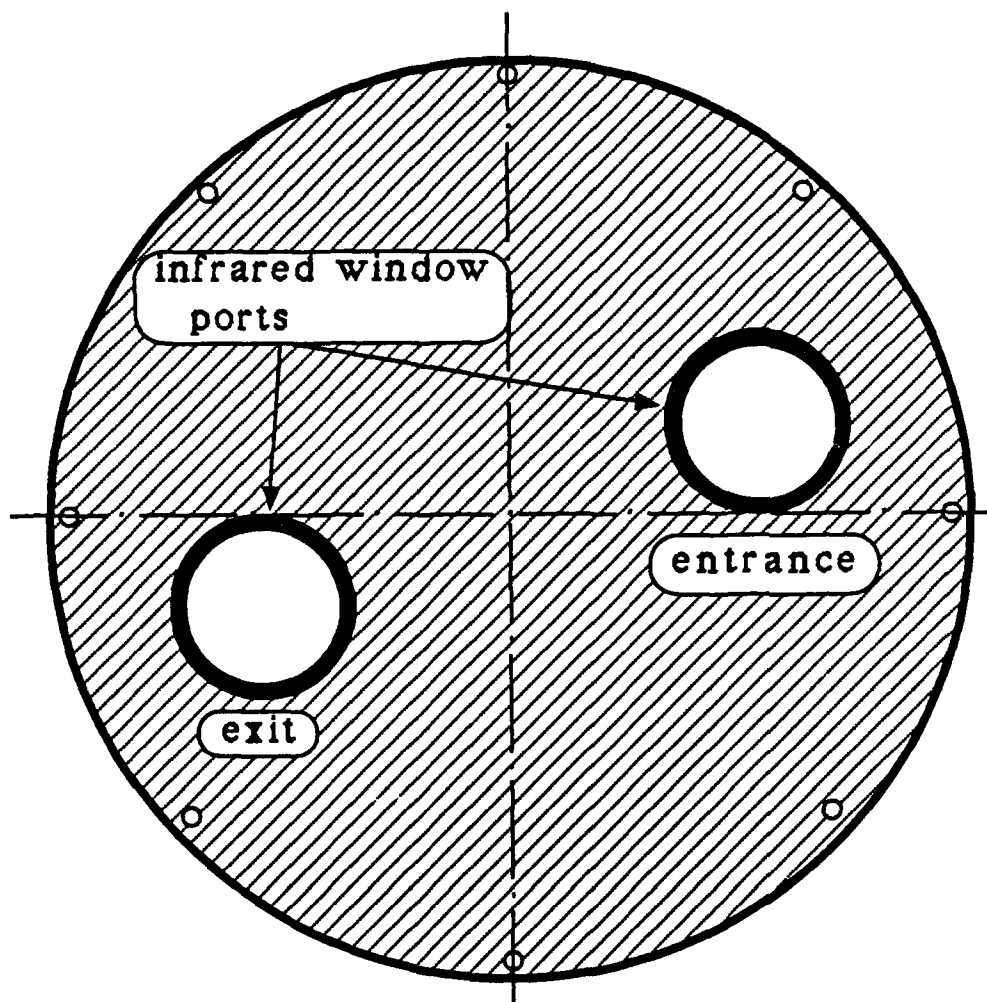


Figure 4. Schematic Drawing Showing the Location of the Infrared Entrance and Exit Windows in the Optical Port Cover Plate (at the In-Focus Location)

A support shelf for the infrared transfer optics and the detector consists of a 20-inch by 24-inch by 1/8-inch piece of stainless steel welded to the chamber wall 3-inch below and centered under the in-focus optical port. This shelf is supported by two 1-inch by 15-inch by 1/8-inch stainless steel side struts welded to the chamber wall and to the shelf. The shelf is enclosed in a 1/8-inch acrylic box to facilitate purging with pure, dry air.

A support frame for the gas handling system and various instruments is fabricated from 1/2-inch aluminum rod (see Figure 2). It measures 24-inches by 24-inches and has two vertical and two horizontal rods in the center to give a 3 by 3 grid of 8-inch squares. The frame has a 12-inch rod welded at each corner perpendicular to the main frame members. These rods extend into the mounting pieces on the chamber and are secured with set screws.

## 2. Temperature Measurements

Three temperature sensors are mounted at different locations on the surface of the chamber; one near the top center, one on the sample stub end, and one near the in-focus mirror stub end. The sensors are K-type (chromel-alumel) thermocouples made from flat foil wire elements (Omega Engineering, Inc., Cat. No. CO2-T). They are placed over an insulating layer of Kapton® adhesive tape and then protected by an additional layer of Kapton tape. One K-type Teflon®-coated thermocouple probe (Omega Engineering, Inc., Cat. No. CASS-18G-12-PFA) is press-fit mounted in 1/4-inch FEP tubing, then extends into the chamber (12 inches) and is held in place with a 1/4-inch stainless steel O-ring compression fitting (Cajon, Ultra-Torr® which provided a vacuum-tight mounting. The final sensor is a K-type air temperature probe (Omega Engineering, Inc., Cat. No. SDX-SET-AP-K-SMP) mounted directly over the chamber to give room temperature readings.

These five probes terminate in a ten-position, two-pole rotary selector switch (Omega Engineering, Inc., Cat. No. OSW3-10). The selected probe output is directed to the input of a microprocessor-based thermocouple meter (Omega

Engineering, Inc., Model 680-S1). The meter produces an ASCII output which is sent over a standard RS-232 line to the FT-IR data system.

The temperature of the chamber is controlled with a recirculating heater/cooler (Neslab Instruments, Inc., Model HX-150DD) using ethylene glycol as the working fluid. The temperature range of the this unit is 5-50 °C. The exterior of the chamber is covered with 1-1/2-inches of high-density foam insulation (Rubatex®) to minimize temperature variations.

### 3. Humidity Measurements

A thin-film humidity probe (Vaisala, Inc., Model HMP 144Y) is mounted in one of the 1/2-inch NPT pipe thread openings in the chamber. The protective fritted metal cover is removed to prevent potential catalytic activity with samples in the chamber. The output voltage from the humidity probe is sent to a digital voltmeter with an RS-232 port (Goertz-Metrawatt, Model M 2110) and from there to the FT-IR data system.

### 4. Pumping System

The chamber is connected from one of the 2-inch KF half nipples with a 2-inch bellows-seal vacuum valve (Airco-Temescal, Cat. No. 1110) to a turbomolecular pumping station (Leybold-Heraeus Vacuum Products, Inc., Model TMV 10,000) through a 4-liter in-line, stainless steel liquid nitrogen trap (Nor-Cal Products, Inc., Model FTN-8-2002). The turbomolecular pumping station includes a 7.0 cfm mechanical pump (Leybold-Heraeus Model D8A), and a 150 liter/sec turbomolecular pump (Leybold-Heraeus Model TMP150).

### 5. Pressure Measurements

A number of different gauges are used to measure the pressure in the chamber. Pressures from 1 torr to 1000 torr are measured with a Bourdon gauge (Wallace & Tiernan Model 61B-1D-0800). Pressures from  $10^{-3}$  torr to 1.0 torr are measured in the chamber with a thermocouple gauge (Teledyne Hastings-Raydist Model VH-3) and at the roughing pump with a second thermocouple gauge (Leybold-

Heraeus Model THERMOVAC TM 220). Pressures from  $10^{-6}$  -  $10^{-3}$  torr are measured with a Penning gauge (Leybold-Heraeus Model PENNINGVAC PM 310). The Penning gauge is mounted with an in-line butterfly shut off valve to one of the 2-inch KF half-nipples on the chamber. The Bourdon gauge is connected to the other KF through a reducing joint.

## 6. Optical System

The optical system consists of three sections: the Fourier transform infrared (FT-IR) spectrometer, the interface optics, and the in situ chamber optics. The optical layout can best be understood by referring to the schematic diagram shown in Figure 5. The collimated output beam from the FT-IR source (S) impinges on a spherical mirror (M7) which focuses an image of the source on a point adjacent to the nesting mirror (M12). The beam is directed to this point by three flat mirrors (M8, M9, and M10) to allow for the relative positions of the chamber and the spectrometer. The beam makes several passes through the chamber and then falls on a spherical mirror (M14) and is focused onto a narrow-band liquid nitrogen cooled, mercury-cadmium-telluride (MCT-A) detector (D).

The interior of the chamber contains a set of five mirrors arranged in a multiple-pass configuration (Reference 6). Four of the mirrors are cut from a single 2-inch thick piece of optical Pyrex® glass 11-inches in diameter. Before the individual mirrors were cut, the circular blank glass section was ground into a spherical mirror with a radius of curvature of 1.00 meter and a figure accuracy of  $1/4$  wave. The two out-of-focus mirrors are circular and have a diameter of 4 inches. The nesting mirror is a 7-inch by 4-inch rectangle with a 1-inch by 1-inch piece removed from one corner. The other mirror from this common glass section is a 1.4-inch by 1-inch rectangle, which was also cut to a thickness of  $1/4$  inch. These mirrors are shown as they were laid out on the glass blank in Figure 6. The fifth mirror is a flat, 1.4-inch by 1-inch section which is also  $1/4$ -inch thick. The reflecting surface of each mirror was given a "double" or enhanced gold coating (all optical fabrication and coating was done by Keim Precision Mirrors, Burbank, CA).

## TOP VIEW

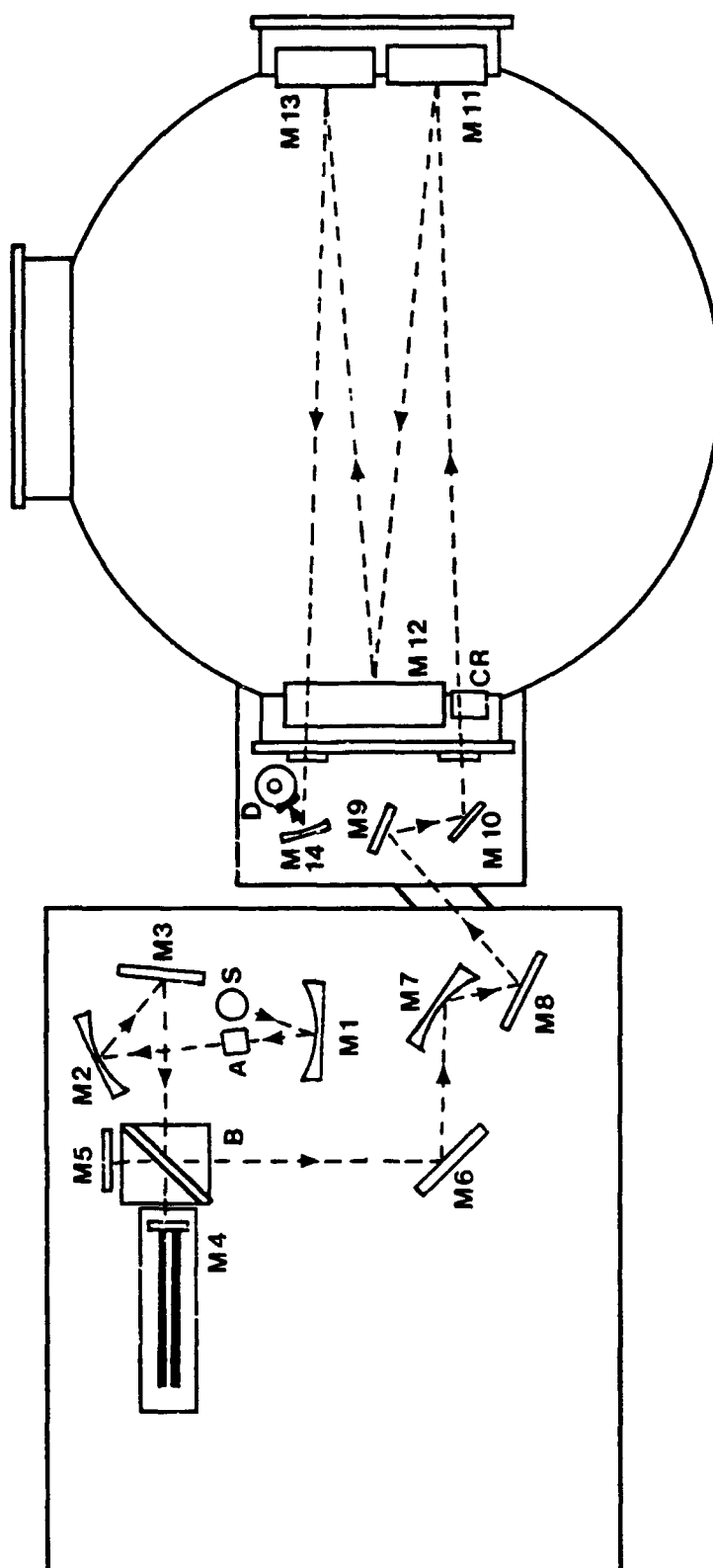


Figure 5. Schematic Drawing of the Relative Positioning of the FT-IR Spectrometer and the Chamber Showing the Optical System and the Path of the Infrared Radiation

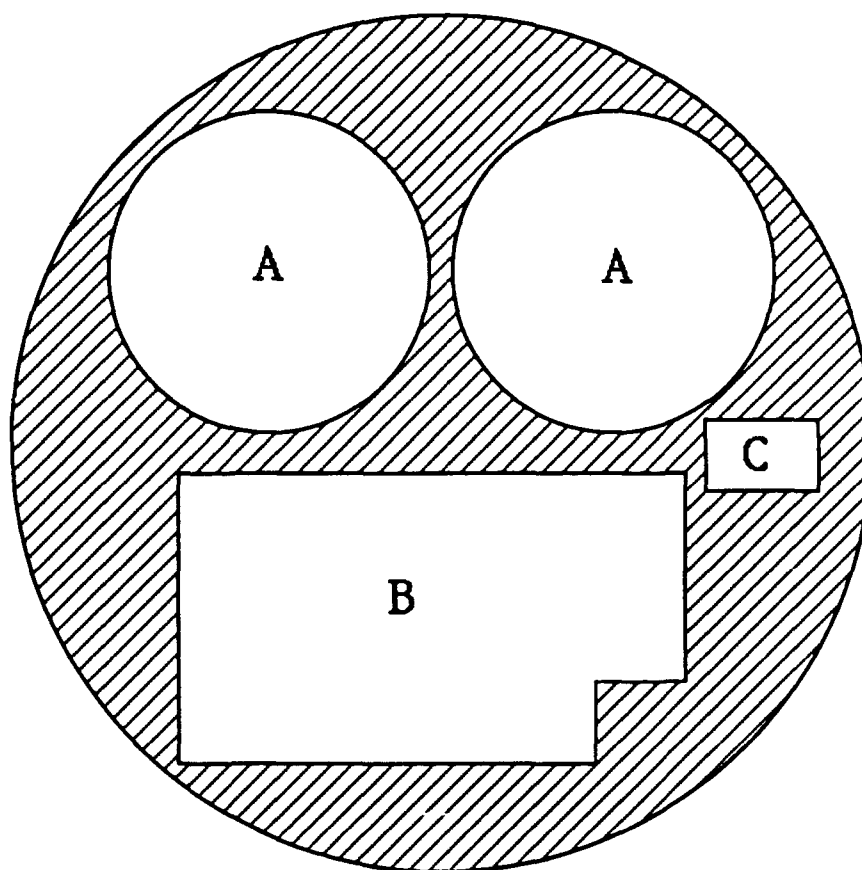


Figure 6. Schematic Drawing of the Pyrex® Mirror Blank from which the Multipass Optical Mirrors were Cut.



The two out-of-focus mirrors are mounted with Teflon®-coated aluminum L brackets and Nylon® set screws to 4-inch square kinematic mirror mounts (Newport Corp., Model 600A-4R) (see Figure 3). The nesting mirror is mounted on a similar kinematic mount (Newport Corp., Model 600A-1). It is secured to the kinematic mount in a similar fashion with four aluminum-coated L brackets and Nylon® set screws. A view of this mirror and the corner reflector mirrors is shown schematically in Figure 7.

The two 1.4-inch by 1-inch mirror sections are glued to a right-angle aluminum support piece with epoxy (Varian Associates, Torr Seal). This piece is welded to a 1/2-inch aluminum rod, then mounts at right angles to a second rod, which is, in turn, welded to a U-shaped aluminum piece, pushed over the fixed mounting bracket in the chamber. This assembly is shown in Figure 8. These two mirrors form the corner mirror assembly introduced by Horn and Pimentel (Reference 7). This modification doubles the useable path length of the original multipass cell described by White (Reference 8).

The pattern of images formed on the nesting mirror using the Horn and Pimentel approach is shown in Figure 9. This Figure illustrates the implementation of the modification suggested by Olsen (Reference 6), and shows the need for offsetting the entrance and exit beam ports. The total number of passes across the chamber is given by the expression (Reference 6):

$$\text{passes} = M(2N-1)-2$$

where M is the number of rows of images on the nesting mirror (four in this system) and N is the number of columns of images on the nesting mirror (fourteen under normal operating conditions). When M is 4 and N is 14, the number of passes is 106, giving a total path length of 106 meters.

All of the kinematic mirror mounts have their vernier adjustment mechanisms replaced with fine-threaded screws and are Teflon® coated. The right angle mirror mount and its support structure are also Teflon® coated.

VIEW FROM INSIDE CHAMBER

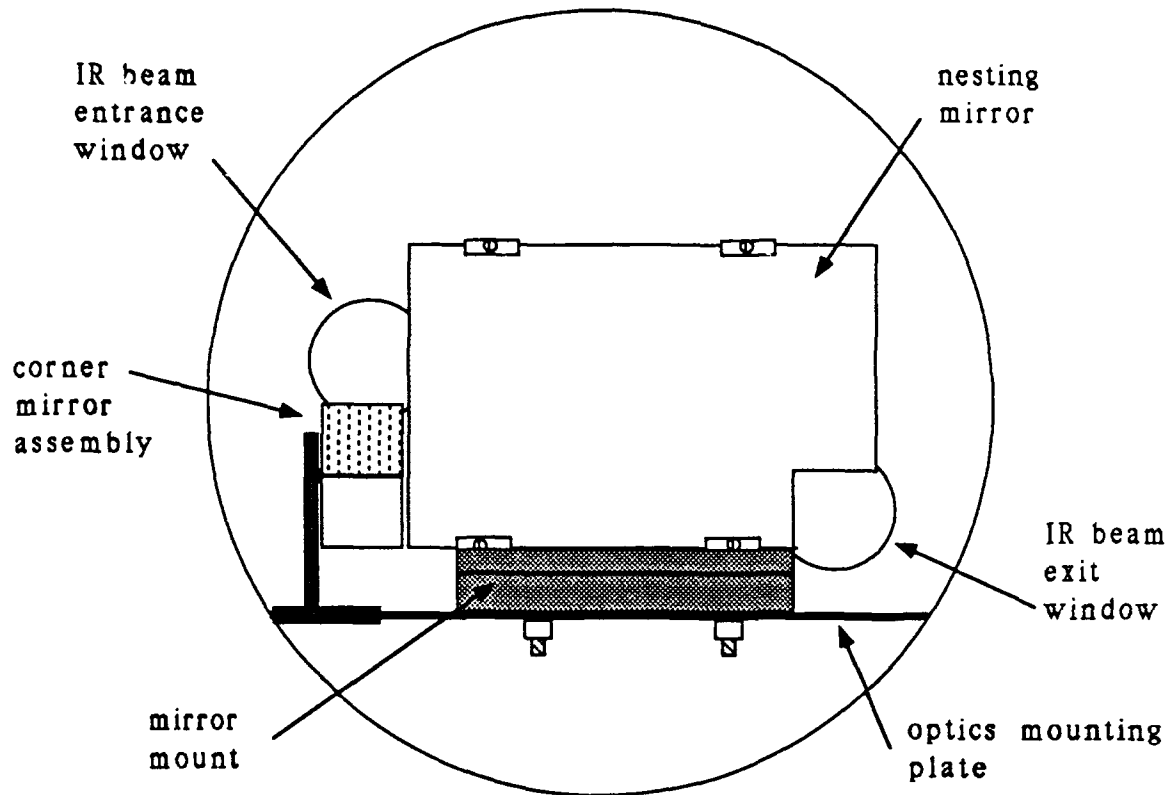


Figure 7. Schematic Drawing of the Nesting Mirror and Corner Mirror Assembly as Mounted in the Chamber (In-Focus Location)

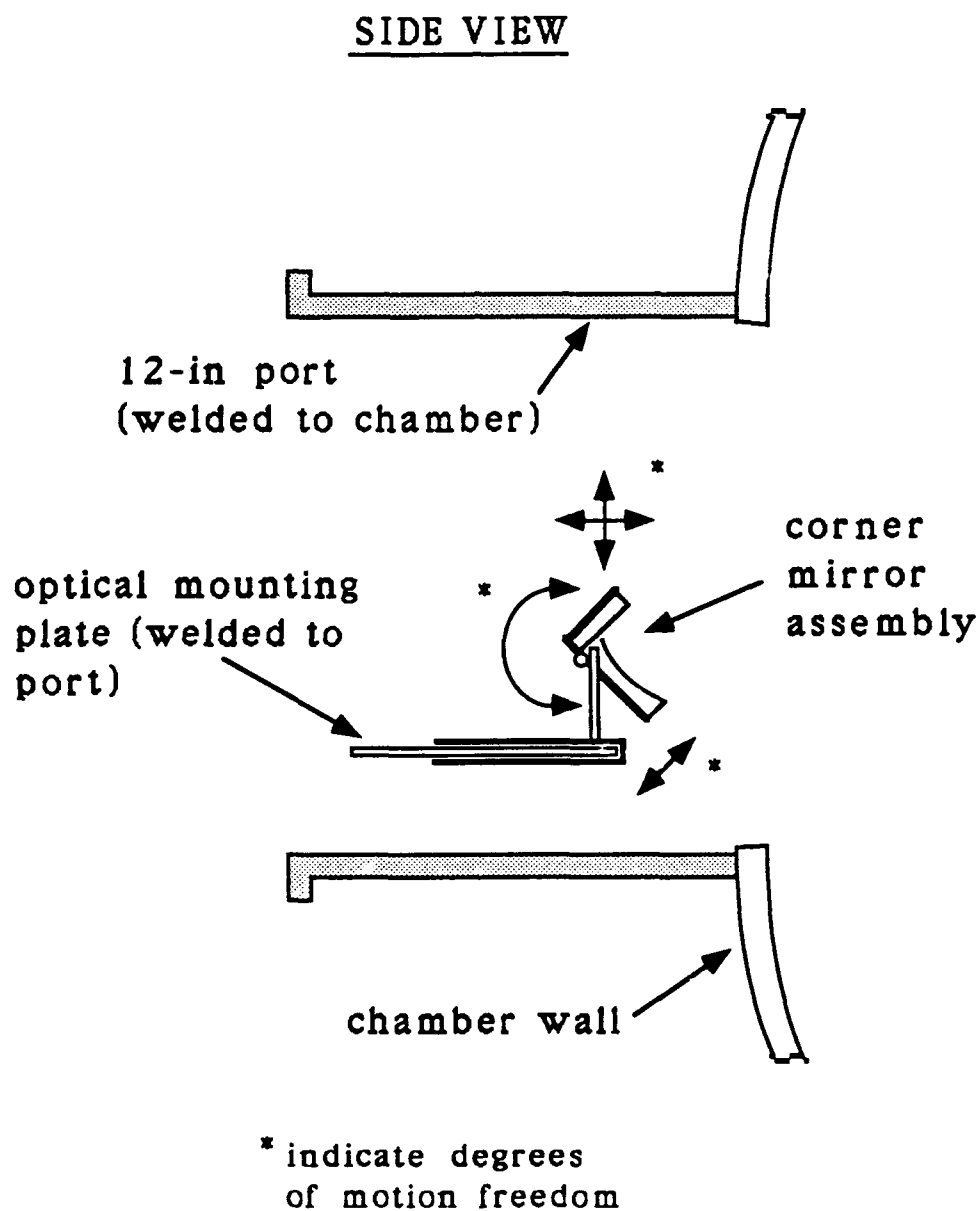


Figure 8. Schematic Drawing of the Corner Mirror Assembly Showing its Mounting Hardware and Degrees of Motion Freedom.

VIEW FROM BACK SIDE OF MIRROR

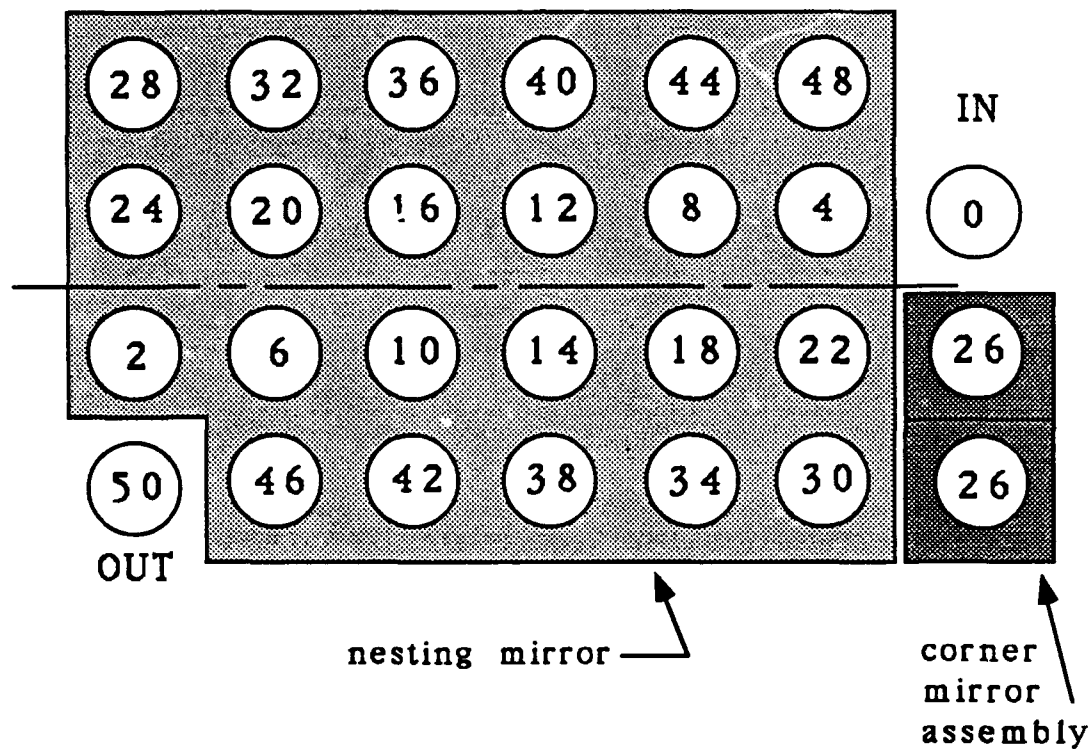


Figure 9. Schematic Drawing of the Nesting Mirror Assembly Showing Locations of Infrared Beam Images in the Multipass Optical System (Set for 50 Passes).

The two beam-steering flat mirrors (A. Jaegers Co., Cat No. 1166) in the external optical interface compartment are 3-inch by 3-inch by 1/4-inch Pyrex® glass. The spherical detector focusing mirror (Gowllands Ltd., Morland Rd., Croydon, UK) is a 3-inch diameter by 1/8-inch thick spherical mirror with a 3-1/2-inch focal length. All of these three mirrors are first-surface type with aluminized reflection surfaces which are overcoated with silicon monoxide. All three of these mirrors are glued with epoxy (Varian Associates, Torr Seal®) to kinematic mirror mounts (Newport Corp., Model MM-2) and screwed to mounting posts with adjustable heights (Newport Corp., Model VPT-4). The mounting posts are secured to base plates (Newport Corp., Model AMB-3) to form a mirror support assembly. These assemblies are secured in place (after adjusting their positions for proper infrared beam direction) with mounts (Newport Corp., Model CL-4) which screw into holes in the chamber external optics table.

The detector is a specially fabricated, extended-length dewar, narrow-band, MCT-A (Infrared Associates, Inc., Model NB FTIR). It is mounted to an adjustable height, Plexiglas® L bracket which is secured to the chamber base plate with a screw-down mount (Newport Corp., Model CL-4).

## 7. Gas-Handling System

A small glass manifold is mounted on the support framework on one side of the chamber. This manifold is shown schematically in Figure 10. It consists of three Teflon® vacuum valves (Kontes, Cat No. 826600-0004) and a mixing bulb. There is also a silicon septum port for sample injections via syringe. The outlet of the manifold proceeds through an additional Teflon® vacuum valve and into the chamber. The entire manifold is wrapped in heating tape to prevent condensation or to evaporate liquid samples.

Samples are introduced into the chamber by direct injection through the silicon septum into the manifold, or by preparation on an external portable vacuum system (shown in Figure 11) with subsequent introduction into the chamber through one of the Teflon® valves.

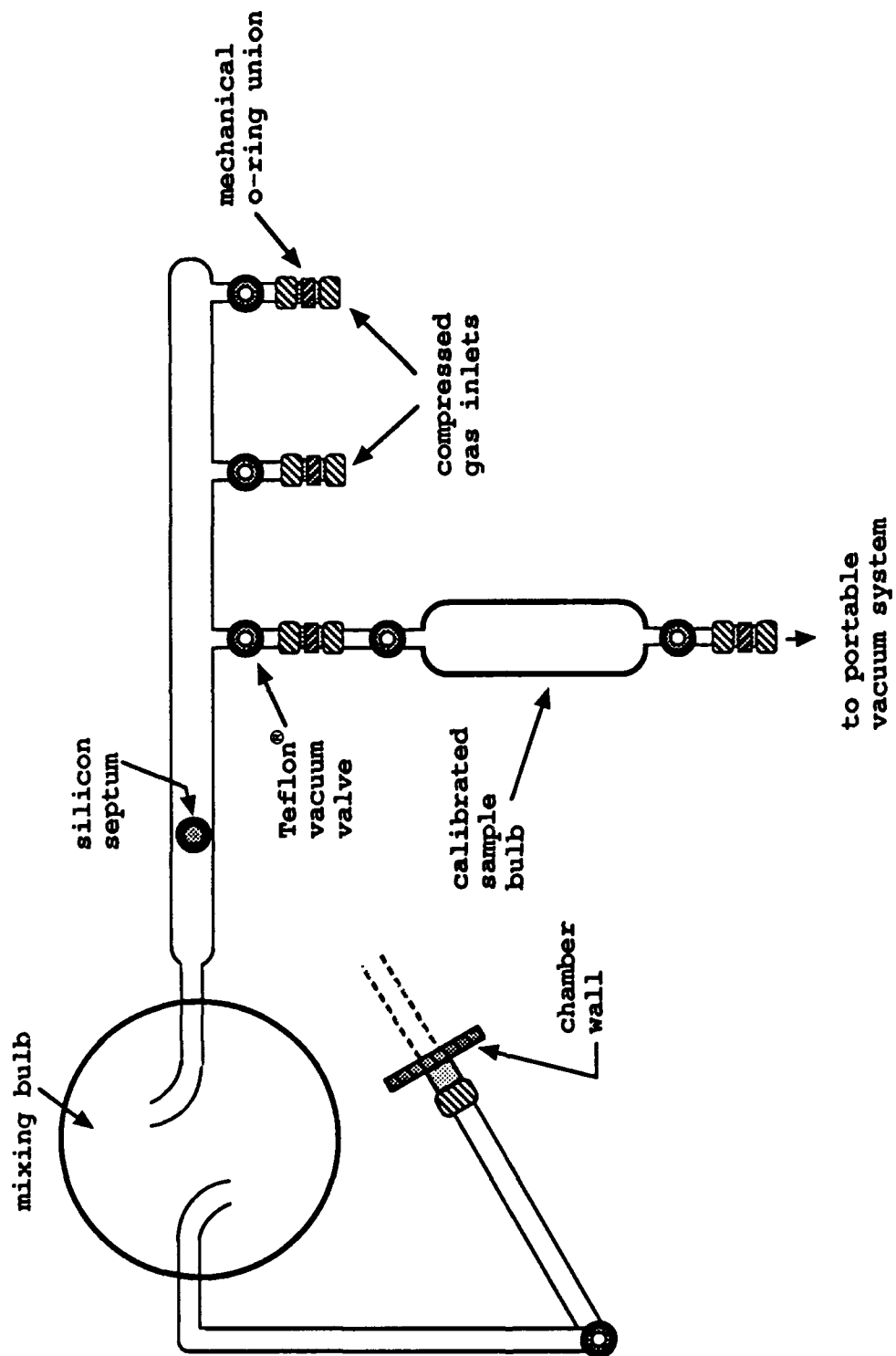


Figure 10. Schematic Diagram of the Chamber Gas Manifold System.

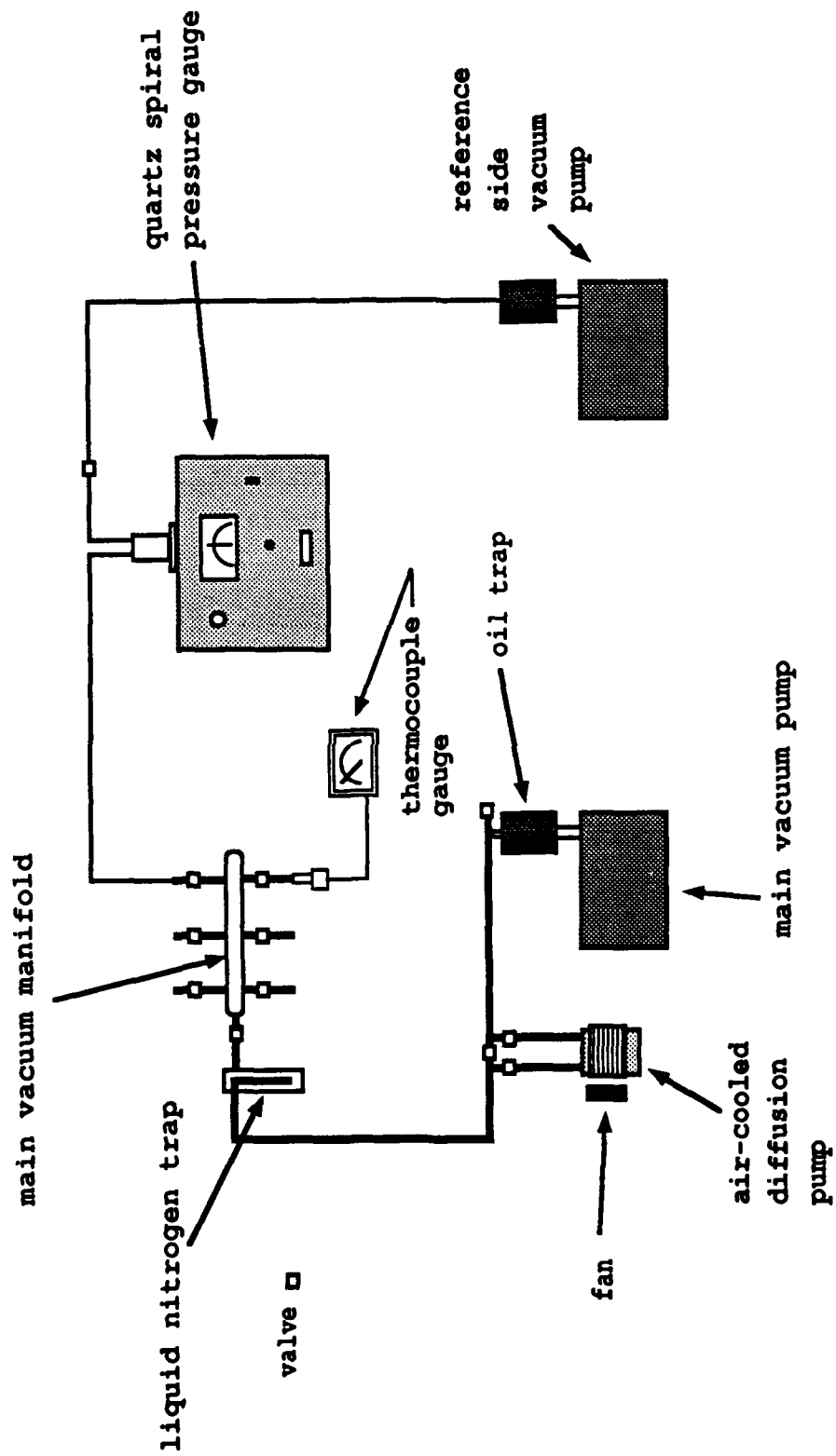


Figure 11. Schematic Drawing of the Portable Vacuum System.

The portable vacuum system consists of a mechanical pump (Sargent-Welch, Model 8815) and an air-cooled diffusion pump (CVC Products, Inc., Model VMF-21) which led through a liquid nitrogen trap to a manifold of eight Teflon® vacuum valves (Kontes, Cat No. 826600-0004). Pressures from  $10^{-3}$  torr to 1.0 torr are measured with a thermocouple gauge (Teledyne Hastings-Raydist, Model VH-3). Vapor samples are prepared by measuring pressures from 1 to 1000 torr with a quartz spiral bourdon gauge (Texas Instruments, Model 145-01). The reference side of the bourdon tube is pumped with a separate mechanical pump (Alcatel Vacuum Products, Model ZM2004). Vapor samples are prepared in glass bulbs with calibrated volumes and Teflon® vacuum valves (Kontes, Cat No. 826600-004) at both ends. They are then introduced into the environmental chamber through a 1/4-inch connecting line of PFA Teflon® tubing.

## 8. Pure Air System

The air used to purge the spectrometer and transfer optics, to supply the interferometer air bearing, and to fill the chamber for certain runs is supplied by a special in-house system. It consists of a standard 15 hp air compressor (Ingersoll-Rand, Type 30, Model 05E 3) supplying compressed air to an air-cooled after cooler (Zeks Air Drier Corp., Model No. 35-ACHA-100) then a prefilter/moisture separator (Wright-Austin, Type 31L-ST-2) with an integral heater to prevent condensate freezing. The compressed air then goes to a dual-tower, pressure swing, heatless dryer (Zeks Air Drier Corp., Model 20MPS3FLO) with a coalescing prefilter and a particulate-removal postfilter. The prefilter drain and the moisture separator drain are connected to an electronically timed valve which expels waste condensate every 15 minutes. The main compressor tank is similarly connected to a separate electronic valve and water condensate is expelled every 5 minutes.

With this arrangement, air at a pressure dew point of  $-74^{\circ}\text{C}$  enters the laboratory. It is then passed through a catalytic air purifier (Aadco, Model 737-15A) to remove any residual hydrocarbons. The resulting air stream is particulate free with a dew point of  $-74^{\circ}\text{C}$  and a hydrocarbon content of less than one part-per-billion. The capacity of the pure air system is 250



liters  $\text{min}^{-1}$ . The layout of the pure air system is shown schematically in Figure 12.

The physical layout of the chamber, the FT-IR system, the portable vacuum system, the chamber vacuum system, and the chamber heating/cooling system is shown in Figure 13.

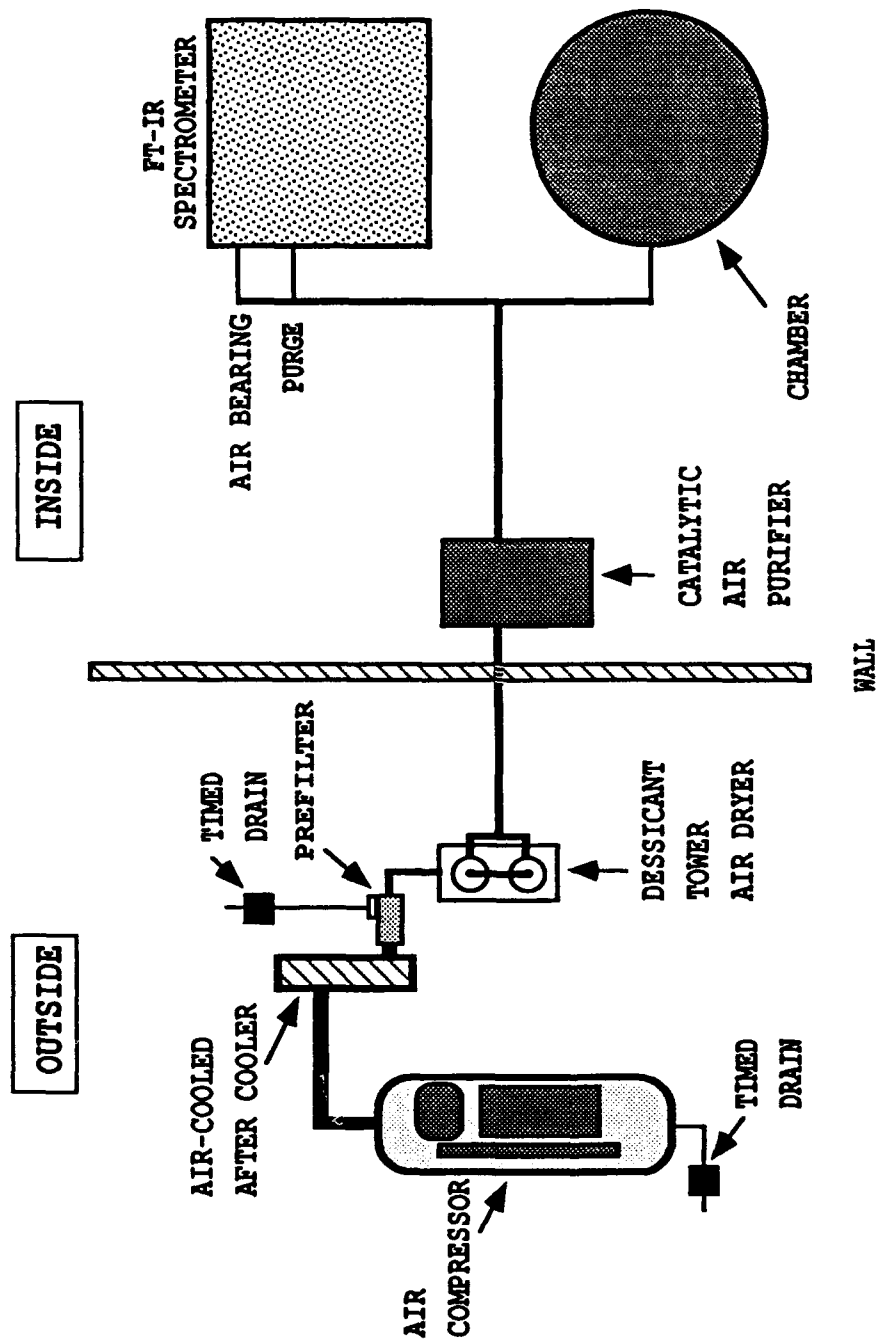


Figure 12. Schematic Diagram of the Pure Air System.

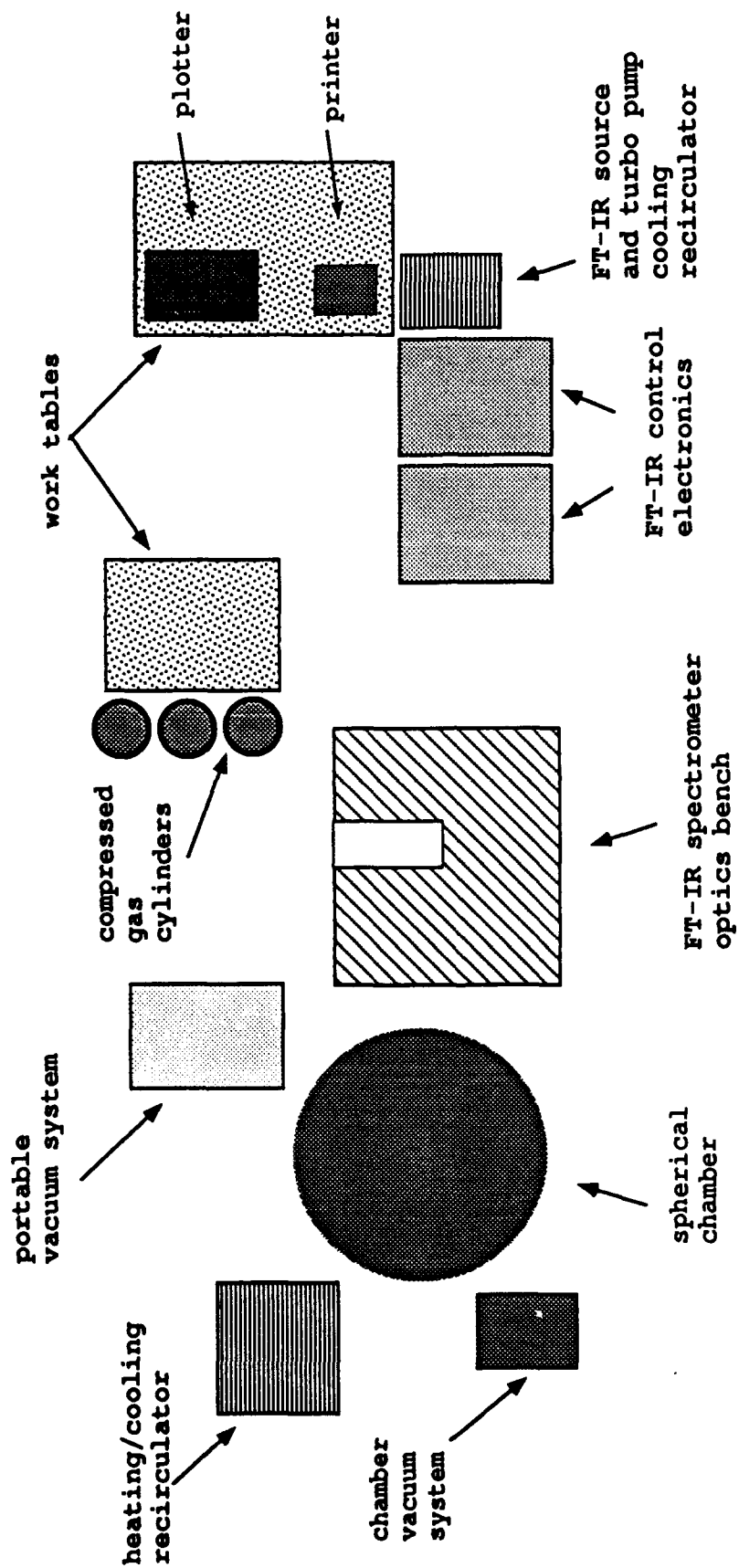


Figure 13. Schematic Diagram of the Chamber and the FT-IR Spectrometer Showing the Relative Locations of the Portable Vacuum System, the Chamber Vacuum System, and the Chamber Heating/Cooling System.

### SECTION III

#### TYPICAL PERFORMANCE CHARACTERISTICS

The chamber has met most of its design criteria, although some operational problems remain. An ultimate vacuum of  $5 \times 10^{-6}$  torr can be attained by pumping for 12 hours with the turbopump on and the external trap filled with liquid nitrogen. A working vacuum of  $8 \times 10^{-5}$  torr can be obtained in 1-2 hours from one atmosphere in the chamber with the turbo pump on (below 1 torr) and no liquid nitrogen in the trap. From an initial vacuum of  $1 \times 10^{-5}$  torr, the chamber has a typical leak rate of about 40 millitorr per day.

The chamber can be filled from an evacuated condition to 760 torr in 6-12 minutes depending on the fill gas; helium is fastest, air or nitrogen is slower. Helium is often used to create synthetic atmospheres because it fills faster and pumps out faster.

The temperature is stable to  $\pm 1$  °C from 6.4 °C to 46.6 °C at any point on the main body of the chamber. However, it is a few degrees warmer or colder at the optical, sample and view ports because they are not insulated and are only cooled or heated by conduction. It takes about four hours to go from one temperature extreme to the other.

Optical stability is adequate, but improvements in coupling the mirror controls through the vacuum port covers are being considered. Path length changes are not a problem, but deterioration of the infrared signal occurs under some conditions because of slight shifts in mirror alignment.

The stability of inert gases in the chamber is very good. There was no discernible loss of methane at 20 ppm in helium in the chamber over a 34-day period as shown in Figure 14 even though there were considerable variations in concentration over that time period. These variations are due, for the most part, to the variations in the peak-to-baseline absorbance measurements taken

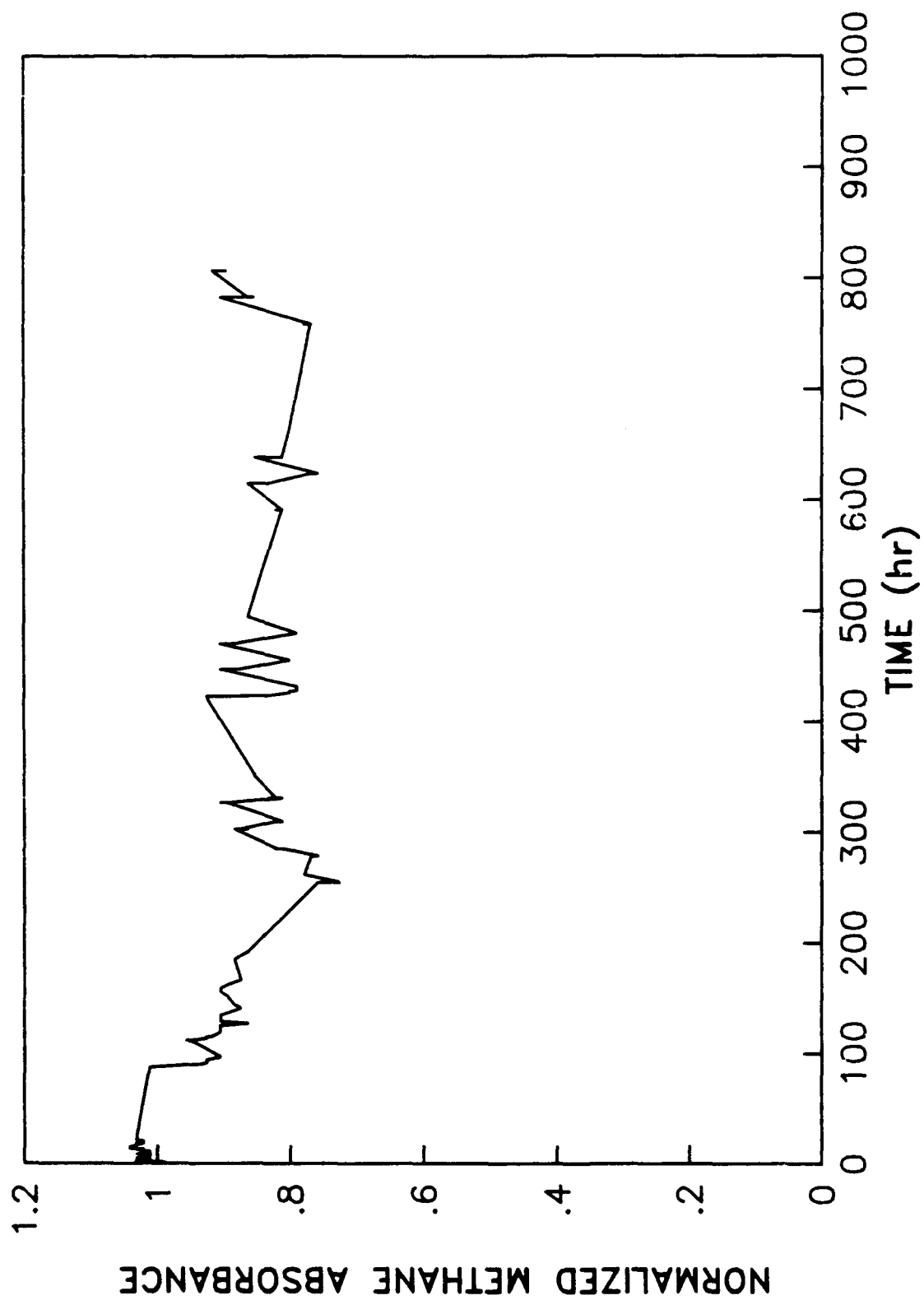


Figure 14. Plots of Methane Stability in the Chamber.

at  $1.0\text{ cm}^{-1}$ . At long path lengths, absorbance values for sharp spectral features tend to vary somewhat, so this behavior is not unexpected.

The stability of hydrazine in the chamber was worse than expected, particularly in the presence of oxygen. This finding will be the subject of another separate publication. The first series of decay curves for hydrazine in dry helium are shown in Figure 15. There was a dramatic conditioning effect evident in this first series of runs. Subsequent hydrazine decay experiments in dry helium have shown some conditioning but have generally been similar to runs 2-4 of figure 14.

Because of this decay behavior, hydrazine stability patterns in the chamber under dry, oxygen-free conditions are being carefully characterized so that a firm baseline can be established for further study of the effects of oxygen, added surfaces, temperature, pressure, etc.

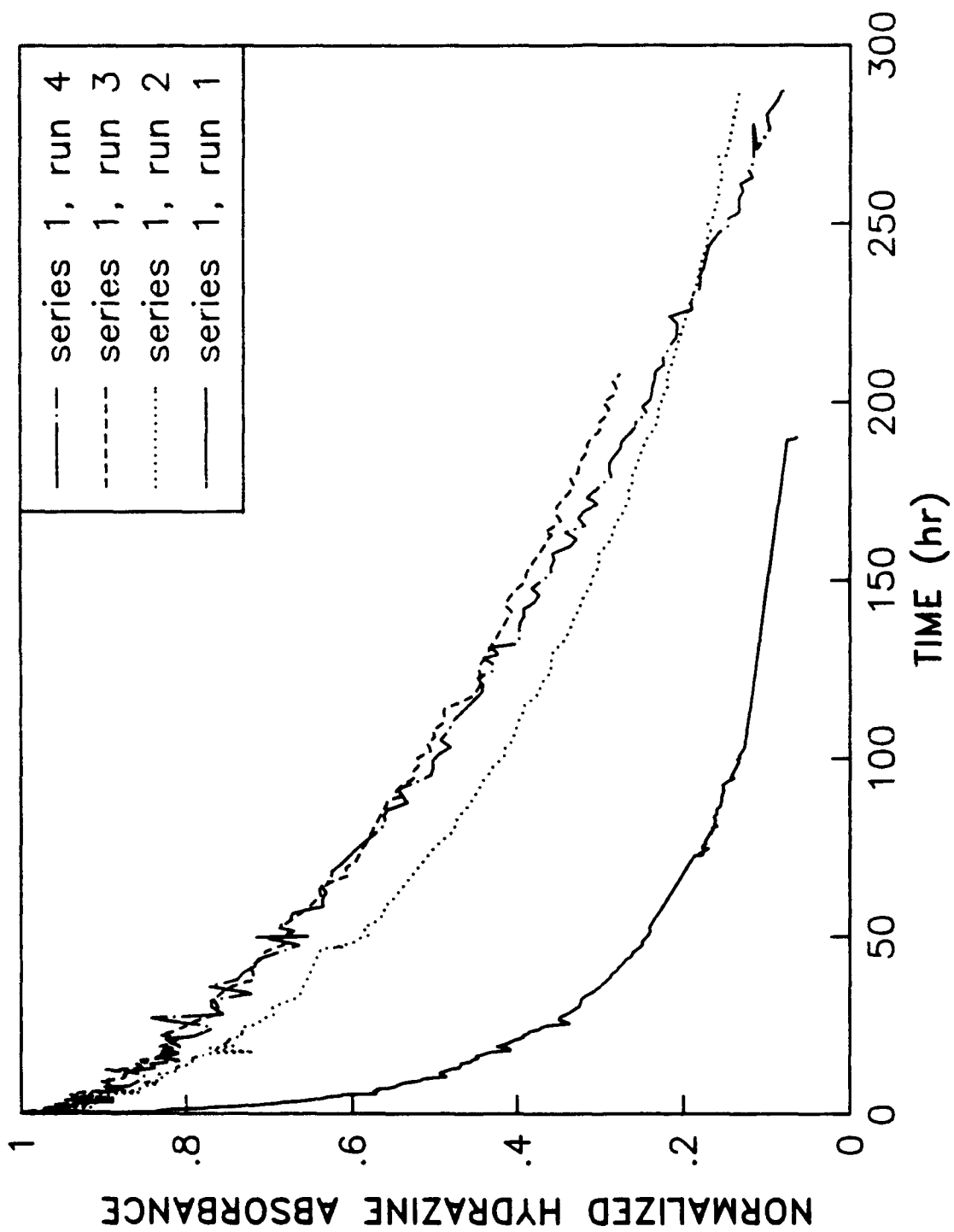


Figure 15. Plots of Hydrazine Stability in the Chamber.

## SECTION IV

### FUTURE PLANS

Considerations are now being given to the addition of a residual gas analysis system to the chamber. This system would be configured to allow leak detection at low pressures, and individual gas component identification at pressures up to one atmosphere. This would be particularly helpful for quantifying oxygen and nitrogen concentrations (which cannot be measured in the mid-infrared) and water concentration. In addition, such a system would be a powerful adjunct to the FT-IR system in the identification of reaction products in more complex mixtures of materials.

Another possible addition would be an artificial sunlight source with a high-power xenon lamp so that photochemical reactions could be studied.



## SECTION V

### CONCLUSIONS

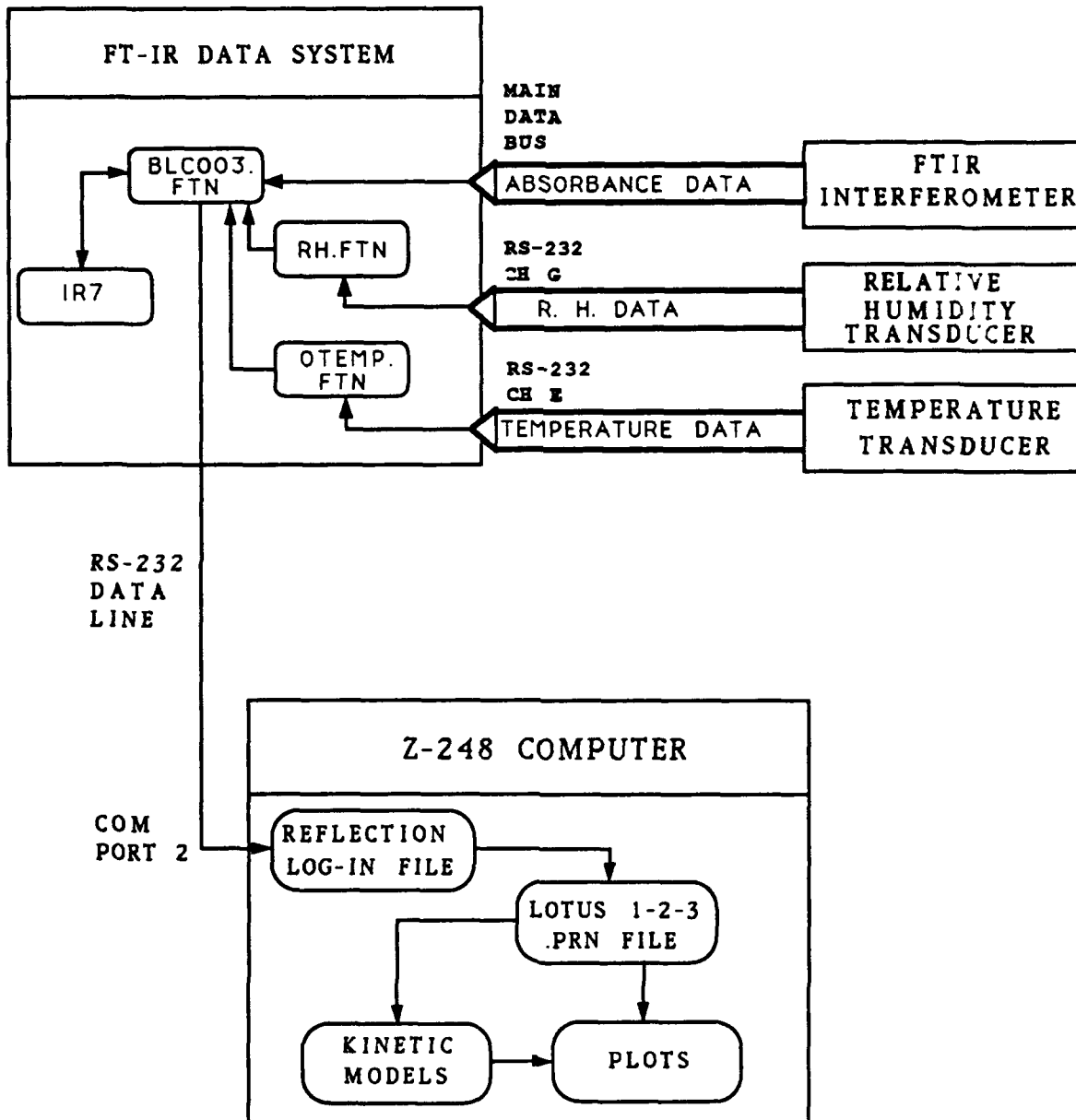
The controlled-environment chamber herein described provides a valuable new platform for the characterization of vapor-phase reactions of toxic chemicals. It enables the effects of temperature, pressure, humidity, and exposure to foreign surfaces to be recorded as a function of time. This will allow experimenters to collect kinetic information which will assist in the prediction of the environmental fate of such chemicals.

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2. D. A. Stone, The Autoxidation of Hydrazine Vapor, CEEDO-TR-78-17, Civil and Environmental Development Office, Tyndall Air Force Base, FL, January 1978.
3. D. A. Stone, The Autoxidation of Monomethylhydrazine Vapor, ESL-TR-79-10, Engineering and Services Laboratory, Air Force Engineering and Services Center, Tyndall Air Force Base, FL, April 1979.
4. D. A. Stone, The Vapor Phase Autoxidation of Unsymmetrical Dimethylhydrazine and 50-Percent Unsymmetrical Dimethylhydrazine-50-Percent Hydrazine Mixtures, ESL-TR-80-21, Engineering and Services Laboratory, Air Force Engineering and Services Center, Tyndall Air Force Base, FL, April 1980.
5. D. A. Stone, F. L. Wiseman, J. E. Kilduff, S. L. Koontz, and D. D. Davis, "The Disappearance of Fuel Hydrazine Vapors in Fluorocarbon-Film Environmental Chambers. Experimental Observations and Kinetic Modeling," Environmental Science & Technology, Vol. 23, pp. 328-333, 1989.
6. W. B. Olson, "Minimization of Volume and Astigmatism in White Cells for Use with Circular Sources and Apertures," Applied Optics, Vol. 23, pp. 1580-1585, 1984.
7. D. Horn and G. C. Pimentel, "2.5 km Low-Temperature Multiple-Reflection Cell," Applied Optics, Vol. 10, pp. 1892-1898, 1971.
8. J. U. White, "Long Optical Paths of Large Aperture," Optical Society of America, Journal, Vol. 32, pp. 285-288, 1942.

# APPENDIX A

## FLOW DIAGRAM FOR DATA ACQUISITION AND ANALYSIS



## APPENDIX B

### SOFTWARE LISTINGS FOR PROGRAM USED FOR OVERALL CONTROL OF FT-IR DATA ACQUISITION AND STORAGE

This program is called IR3. It was written in the Nicolet MACRO language by using the TED editor and then compiling with the Nicolet utility program MACCRT. This procedure allows remarks to be included in the program for documentation and user assistance.

The main MACRO program (IR3) calls other SUB-MACRO programs. These were written and compiled as subsections of IR3. Each program ends with the statement END. Each new program begins with "!" followed by the program name.

```

!IR3          \ACQUIRES, BASELINE CORRECTS, AND PRINTS OR
/             SENDS SPECTRAL DATA TO A PRINTER OR OPEN
/             COMPUTER FILE. (USES THE FORTRAN
/             PROGRAM BLC003.FTN FOR BASELINE CORRECTION)
/
/             USES A SINGLE, USER-SPECIFIED SAMPLING INTERVAL
/
BFN
DFN
NSD
OMD
ENTER LOTUS-FORMAT DATE (1 JUN 89 = 32660)
RTP
OMD
ENTER THE SPECIES TO MEASURE, YES=1, NO=0
OMD
SPECIES FLAGS ARE: HZ=WTY, MMH=SMN, UDMH=SIZ, CH4=ITR, SF6=MNT
OMD
                  NH3=RTO

WTY
SMN
SIZ
ITR
MNT
RTO
OMD
ENTER THE DELAY TIME (0.1 MIN) BETWEEN SPECTRA
VFO
OMD
PRESS "RETURN" TO BEGIN
PAU
VIO=0
TS2
END
          \\\\\\\

```

```

!TS2          \MACRO TO PERFORM THE DATA ACQUISITION
\             AND PROCESSING
\
FOR AAA=1 TIL 120\ LOOP TO ACQUIRE AND PROCESS 120 FILES
PRN DFN
AQ6\          MACRO TO ACQUIRE AND PRINT DATA
DFN=DFN+1
DL3\          MACRO TO EXECUTE THE DESIRED DELAY
\             BETWEEN SETS OF SCANS
NXT AAA
END           \\\\\\\

```

```

!DL3          \MACRO TO EXECUTE THE DESIRED DELAY
\             BETWEEN SETS OF SCANS (IN 0.1 MIN
\             INCREMENTS)
\             PART OF TS2
\
DCL=204445
DCX
FOR III=1 TIL VFO
FOR AAA=0 TIL 6000
NXT AAA
NXT III
DCL=210414
DCX
END           \\\\\\\

```

```

!AQ6          \MACRO TO ACQUIRE, COMPUTE, AND PRINT OUT A
\             BASELINE-CORRECTED ABSORBANCE VALUE FOR ANY OF THE
\             SPECIES CHOSEN FOR MONITORING. ALSO INCLUDES
\             THE FORTRAN PROGRAMS OTEMP.FTN AND RH.FTN, WHICH
\             ACQUIRE TEMPERATURE AND RELATIVE HUMIDITY DATA
\
TEM=4\        SET TEM TO TOGGLE PRINTER ON
NPR\          TURN ON PRINTER
SCD
GFN
OTEMP.FTN
FRN
GFN
RH.FTN
FRN
OFN=DFN
MOS
RAS
ABS
XSP=4000
XEP=700
YSP=-.25

```

YEP=1.25  
DSS  
XEP=0  
DFN=SFN  
GFN  
BLC003.FTN  
FRN  
TEM=4\SET TEM TO TOGGLE PRINTER OFF  
NPR\TURN PRINTER OFF  
DFN=OFN  
END  
!!

\\\\\\\\\\

## APPENDIX C

## SOFTWARE LISTING FOR FORTRAN PROGRAM USED TO ACQUIRE TEMPERATURE DATA

Data is acquired over a dedicated cable which runs from the Omega Model 680 thermocouple thermometer to the RS-232 data channel G input on the back of the Nicolet 1280 computer.

CCCCCCCCCCCC

## PROGRAM OTEMP.ASC

THIS IS A PROGRAM TO READ ASCII  
TEMPERATURE DATA FROM AN OMEGA MODEL  
680 THERMOCOUPLE THERMOMETER INTO  
THE FT-IR DATA SYSTEM AND STORE THE  
RESULT IN EACH SCRATCH FILE STATUS  
BLOCK IN LOCATIONS 68-71.

## DEFINE VARIABLES

```

INTEGER CHANNEL,BAUDRATE,BIT,BAUDVAL,DELAY,IOUT,I,
1DELTA, VALUE
INTEGER IDATA(512),IT4,IT5,IT6,IT7
LOGICAL VALID
REAL R1
CHARACTER*4 TT
CHARACTER*10 TMP(10),WT
CHARACTER*1 CHR,T1,T2,T3,T4,T5,T6,T7

```

FLASER=15798.2  
NPMAX=22528

C  
C  
C

READ FT-IR PARAMETERS FOR DATA RETRIEVAL

```
IDFN=IRVAL(14022,0)
NSECS=IRVAL(14001,0)
INODE=IRVAL(13004,0)
NDPW=IRVAL(14000,0)
IXSP=IRVAL(14025,0)
IENP=IRVAL(14026,0)
```

C  
C  
C

LOCATE SECTORS TO BE READ USING THE FOLLOWING INDEX

$$\text{IDFSEC} = (\text{IDFN} + 1) * \text{NSECS} + 87$$

C  
C  
C  
C

READ HEADER BLOCK INFORMATION USING IRTISK. STORE RESULTS IN AN ARRAY CALLED IDATA.

CALL IRTISK(IDATA,512,IDFSEC,INODE)

C

```

C  SET BAUDRATE AT 1200, CHANNEL=2 (I.E., CHANNEL G)
C  AND CALL SUBROUTINE BAUDSET
    BAUDRATE=1200
    CHANNEL=2
    VALID =.TRUE.
    CALL BAUDSET(CHANEL, BAUDRATE, VALID)

C  SEND CHARACTER "R" TO REQUEST DATA TRANSMISSION FROM THE
C  OMEGA UNIT
    VALUE = 82
    CALL CHWRITE (CHANNEL,VALUE,VALID)

C  RECEIVE THE CHARACTERS TRANSMITTED BY THE OMEGA UNIT
    DELAY=0
    DO 10 I=1,8
        CALL CHREAD(CHANNEL,DELAY,CHR,VALID)
        TMP(I)=CHR
10  CONTINUE

    T1=TMP(1)
    T2=TMP(2)
    T3=TMP(3)
    T4=TMP(4)
    T5=TMP(5)
    T6=TMP(6)
    T7=TMP(7)

C
C  WRITE THE INDIVIDUAL TEMPERATURE CHARACTERS TO LOCATIONS
C  68-71 OF THE IDATA ARRAY
C
    IDATA(68)=ICHAR(T4)
    IDATA(69)=ICHAR(T5)
    IDATA(70)=ICHAR(T6)
    IDATA(71)=ICHAR(T7)

    CALL IWTISK(IDATA,512,IDFSEC,INODE)
    CALL EXIT
    END

```



## APPENDIX D

### SOFTWARE LISTING FOR FORTRAN PROGRAM USED TO ACQUIRE HUMIDITY DATA

Data is acquired over a dedicated cable which runs from the M2110 digital voltmeter (which receives humidity data from the Vaisala HMP 114Y transducer) to the RS-232 channel E on the back of the Nicolet 1280 computer.

C  
C  
C  
C  
C  
C  
C  
C  
C  
C  
C  
C  
C  
C  
C

#### PROGRAM RH.ASC

PROGRAM TO READ ASCII RELATIVE  
HUMIDITY DATA FROM A VAISALA MODEL  
HMP 114Y TRANSDUCER INTO THE FT-IR  
DATA SYSTEM AND STORE THE RESULTS IN  
EACH SCATCH FILE STATUS BLOCK IN  
LOCATIONS 238-243.

#### DEFINE VARIABLES

INTEGER CHANNEL, BAUDRATE, BIT, BAUDVAL, DELAY, IOUT, I,  
IDELTA, VALUE  
INTEGER IDATA(512), IH3, IH4, IH5, IH6, IH7  
LOGICAL VALID  
REAL R1  
CHARACTER\*6 H  
CHARACTER\*10 HUMID(10)  
CHARACTER\*1 CHR, RH1, RH2, RH3, RH4, RH5, RH6, RH7

FLASER=15798.2  
NPMAX=22528

C  
C  
C

#### READ FT-IR PARAMETERS FOR DATA RETRIEVAL

IDFN=IRVAL(14022,0)  
NSECS=IRVAL(14001,0)  
INODE=IRVAL(13004,0)  
NDPW=IRVAL(14000,0)  
IXSP=IRVAL(14025,0)  
IENP=IRVAL(14026,0)

C  
C  
C

#### LOCATE SECTORS TO BE READ USING THE FOLLOWING INDEX

IDFSEC=(IDFN+1)\*NSECS+87

C  
C  
C  
C

READ HEADER BLOCK INFORMATION USING IRTISK. STORE  
RESULTS IN AN ARRAY CALLED IDATA.

CALL IRTISK(IDATA,512,IDFSEC,INODE)

C

```

C  SET BAUDRATE AT 1200, CHANNEL=2 (I.E., CHANNEL G)
C  AND CALL SUBROUTINE BAUDSET
    BAUDRATE=1200
    CHANNEL=1
    VALID =.TRUE.
    CALL BAUDSET(CHANNEL, BAUDRATE, VALID)

C  SEND CHARACTER "ENQ" TO REQUEST DATA TRANSMISSION FROM THE
C  M2110 UNIT
    VALUE = 5
    CALL CHWRITE (CHANNEL,VALUE,VALID)

C  RECEIVE THE CHARACTERS TRANSMITTED BY THE M2110 UNIT
    DELAY=0
    DO 10 I=1,7
        CALL CHREAD(CHANNEL,DELAY,CHR,VALID)
        HUMID(I)=CHR
10  CONTINUE

C  SET VALUES OF RH1-RH7 FROM INPUT DATA
    RH1=HUMID(1)
    RH2=HUMID(2)
    RH3=HUMID(3)
    RH4=HUMID(4)
    RH5=HUMID(5)
    RH6=HUMID(6)
    RH7=HUMID(7)

C
C  WRITE THE INDIVIDUAL TEMPERATURE CHARACTERS TO LOCATIONS
C  238-243 OF THE IDATA ARRAY
C
    IDATA(238)=ICHAR(RH1)
    IDATA(239)=ICHAR(RH4)
    IDATA(240)=ICHAR(RH5)
    IDATA(241)=ICHAR(RH3)
    IDATA(242)=ICHAR(RH6)
    IDATA(243)=ICHAR(RH7)

    CALL IWTISK(IDATA,512,IDFSEC,INODE)
    CALL EXIT
    END

```

SOFTWARE LISTING FOR FORTRAN PROGRAM USED TO PROCESS  
AND SEND CHAMBER DATA TO AN EXTERNAL COMPUTER FOR ANALYSIS

PROGRAM BLC003.ASC

THIS PROGRAM RETRIEVES DATA FROM FT-IR SCRATCH FILES,  
AND CALCULATES BASELINE-CORRECTED ABSORBANCE VALUES FOR  
ANALYTICAL PEAKS. THERE IS A SUBROUTINE FOR EACH  
SPECIES OF INTEREST. THERE ARE ALSO SUBROUTINES FOR  
TEMPERATURE AND RELATIVE HUMIDITY DETERMINATIONS.

THIS PROGRAM IS CALLED FROM THE MACRO IR7 AND SENDS  
THE DATA DIRECTLY TO AN OPEN DISK FILE ON A ZENITH  
Z-248 COMPUTER OVER AN RS-232 LINE. FOR EACH SPECTRUM  
ACQUIRED THE OUTPUT DATA HAS THE FORM:

32665 09 15 41 20.3 1.023 .897 .235 05.17

WHERE THE DATA ARE (IN ORDER) - LOTUS-FORMAT DATE, TIME OF  
ACQUISITION OF THE FT-IR FILE (HH MM SS), TEMPERATURE  
(DEG C), ABSORBANCE VALUES (THREE ARE SHOWN), AND %RH.

PROGRAM DIMENSIONED FOR 1.0 CM-1 SPECTRA

REAL Y(16384),BP1,LBP,PXA,PYA,CABS,XDIF,XDIF2,YDIF,  
1FAC1,FAC2,EP,SP,A1,A2,A3,A4,A5,A6  
INTEGER IDATA(512),IDA(22528),COUNT,DP1,DP2,TFLAG,LDATE  
CHARACTER\*2 HH,NN,SS  
CHARACTER\*1 CT1,CT2,CT3,CT4  
CHARACTER\*1 H1,H2,N1,N2,S1,S2  
CHARACTER\*1 RH1,RH2,RH3,RH4,RH5,RH6  
CHARACTER\*4 CTEMP  
CHARACTER\*6 HUMID

FLASER = 15798.2

NPMAX = 22528

SN = 0

\*\*\*\*\*  
READ FTIR PARAMETERS FOR DATA RETRIEVAL:

IDFN = IRVAL(14022,0)  
NSECS = IRVAL(14001,0)  
INODE = IRVAL(13004,0)  
NDPW = IRVAL(14000,0)  
IXSP = IRVAL(14025,0)  
IXEP = IRVAL(14026,0)

IXEP = IRVAL(14026,0)

C  
C THESE IRVAL FUNCTIONS READ THE MEMORY LOCATIONS CORRESPONDING  
C TO THESE PARAMETERS (ALL ARE INTEGERS):

(OCTAL) LOCATION	PARAMETER
13004	INODE NO.
14000	NDP (=INTEGER/256)
14001	FSZ (=INTEGER/512)
14022	DFN
14025	XSP
14026	XEP

C \*\*\*\*\*

C  
C READ FTIR PARAMETERS FOR SETTING SUBROUTINE FLAGS:  
C (1=HZ, 2=MMH, 3=UDMH, 4=CH4, 5=SF6, 6=NH3)

C  
C IFLAG1 = IRVAL(13710,0)  
C IFLAG2 = IRVAL(13713,0)  
C IFLAG3 = IRVAL(13714,0)  
C IFLAG4 = IRVAL(13715,0)  
C IFLAG5 = IRVAL(13723,0)  
C IFLAG6 = IRVAL(13750,0)

C  
C THESE IRVAL FUNCTIONS READ THE MEMORY LOCATIONS CORRESPONDING  
C TO THESE PARAMETERS (ALL ARE INTEGERS):

(OCTAL) LOCATION	PARAMETER
13710	WTY
13713	SMN
13714	SIZ
13715	ITR
13723	MNT
13750	RTO

C \*\*\*\*\*

C  
C THE FIRST 88 SECTORS OF THE SCRATCH AREA (I.E., SECTORS 0-87)  
C CONTAIN MISCELLANEOUS INFORMATION. SCRATCH FILE 0 BEGINS AT  
C SECTOR 88 AND OCCUPIES FSZ/512 SECTORS. ALL SUBSEQUENT FILES  
C ARE THE SAME SIZE AS FILE 0.

C  
C THE LAST SECTOR OF EACH FILE IS THE FILE STATUS BLOCK. THERE  
C ARE A CONSIDERABLE NUMBER OF SECTORS BETWEEN THE END OF THE  
C DATA AND THE BEGINNING OF THE FILE STATUS BLOCK. IT IS NOT  
C CLEAR WHAT THESE EXTRA SECTORS ARE USED FOR.

C  
C \*\*\*\*\*

C  
C LOCATE SECTORS TO BE READ USING THE FOLLOWING INDEX.

```

C
C      IDFSEC=(IDFN+1)*NSECS+87
C
C *****
C
C READ HEADER BLOCK INFORMATION USING IRTISK.  STORE RESULTS
C IN AN ARRAY CALLED IDATA.
C
C      CALL IRTISK(IDATA,512,IDFSEC,INODE)
C
C NOW, FILE STATUS INFO CAN BE DETERMINED FROM THE ELEMENTS
C OF IDATA:
C      IABS = ABSORBANCE FLAG, 0 IF ABSORBANCE
C      IPTS = NO. OF DATA POINTS
C      FEXP = EXPONENT FOR FILE SCALING
C      FXAX = DATA POINT SPACING ON X AXIS
C
C      IABS = IDATA(10)
C      IF (IABS.NE.0) GOTO 900
C      IPTS = IDATA(15)*128
C      FEXP = 2**(19-IDATA(6))
C      FXAX = FLASER/(IPTS*IDATA(17))
C
C NOW DETERMINE THE STARTING AND ENDING POINTS FOR THE FILE TO
C BE READ.  THIS IS DONE BY TWO SEQUENTIAL IF - ENDIF LOOPS.
C THE FIRST SETS ISTEP EQUAL TO THE LESSER OF XSP AND XEP
C (WHICH ARE READ FROM THE FT-IR SCRATCH FILE HEADER BLOCK).
C THE SECOND LOOP CONVERTS THE XSP AND XEP VALUES FROM CM-1
C TO SCRATCH FILE DATA POINT VALUES.  THE 0.5 FACTOR WHICH IS
C ADDED ENSURES THAT INTEGER ISTEP AND IENP VALUES ARE ROUNDED
C CORRECTLY.
C
C      IF (IXSP.LE.IXEP) THEN
C          ISTEP = IXSP
C          IENP = IXEP
C      ELSE
C          ISTEP = IXEP
C          IENP = IXSP
C      ENDIF
C      IF (IXSP.GT.IXEP) THEN
C          ISTEP = IXEP/FXAX+0.5
C          IENP = IXSP/FXAX+0.5
C      ELSE
C          ISTEP = IXSP/FXAX+0.5
C          IENP = IXEP/FXAX+0.5
C      ENDIF
C      NP = IENP-ISTEP+1
C
C      CHECK FOR A REASONABLE NO. OF PTS. IN NP
C
C      IF (NP.GT.NPMAX) THEN
C          WRITE(2,901) NPMAX,NP

```

```

        ELSEIF (NP.LT.5) THEN
            WRITE(2,902) NP
        ENDIF
C
C NOW READ DATA FROM SCRATCH FILE DFN INTO ARRAY IDA
C
C IN IS A COUNTER. NDONE TAKES THE DATA POINT VALUE OF ISTP AND
C CONVERTS IT TO SECTORS. NSKIP TAKES THE STARTING DATA POINT
C VALUE (ISTP) AND SUBTRACTS AN INTEGER NO. OF DATA POINTS, BY
C SECTOR, FROM IT, LEAVING THE POINT IN THE SELECTED SECTOR
C WHERE DATA REPRESENTING THE INTERVAL ISTP - IENP BEGIN.
C
        IN = 1
        NDONE = ISTP/512
        NSKIP = ISTP-NDONE*512
C
C IF THE SCRATCH FT-IR FILE HAD XSP=0 OR XEP=0, THEN DATA CAN
C BE READ DIRECTLY, ONCE THE PROPER BEGINNING SECTOR IS
C SPECIFIED. IF XSP OR XEP WERE NOT ZERO, THEN NDONE SECTORS
C PLUS NSKIP POINTS MUST BE SKIPPED OVER TO BEGIN READING DATA.
C
C RESET FLAG FOR BASELINE CORRECTION ROUTINE
C
        IFLAG=0
        IF (NSKIP.GT.0) THEN
C
C SET FLAG FOR BASELINE CORRECTION ROUTINE
C
            IFLAG=1
            CALL IRTISK(IDA,512,88+IDFN*NSECS+NDONE,INODE)
            DO 20 I=NSKIP+1,512
                IDA(IN) = IDA(I)
                IN = IN + 1
            20 CONTINUE
            NDONE = NDONE + 1
        ENDIF
C
C NPREM IS A COUNTER WHICH TELLS HOW MANY DATA POINTS TO READ
C FROM THE FT-IR SCRATCH FILE TO COVER THE INTERVAL SPECIFIED
C BY ISTP AND IENP.
C
        NPREM = NP-IN+1
        IF (NPREM.GT.0) THEN
            CALL IRTISK(IDA(IN),NPREM,88+IDFN*NSECS+NDONE,INODE)
        ENDIF
C
C NOW THE POINTS IN THE INTEGER ARRAY IDA ARE CONVERTED TO REAL
C VALUES BY DIVIDING EACH ONE BY FEXP (SEE FT-IR SOFTWARE
C MANUAL, P. 18-5 FOR AN EXPLANATION). NOTE THAT ANY TOTALLY
C ABSORBING DATA POINTS HAVE THE VALUE -524288 AND THESE ARE
C SET EQUAL TO ZERO IN THE REAL DATA ARRAY.
C

```

```

      DO 50 I = 1,NP
        IDAS = IDA(I)
        IF (IDAS.EQ.-524288) IDAS = 0
        Y(I) = IDAS/FEXP
50    CONTINUE
C
C *****
C NOW THAT THE DATA POINTS ARE AVAILABLE, BASELINE CORRECTION
C CAN BE MADE. THE CORRECTION WILL BE MADE IN THE SAME MANNER
C IT WOULD BE DONE BY HAND. A POINT ON ONE SIDE OF THE
C ANALYTICAL PEAK WILL BE CHOSEN BY AVERAGING THE ABSORBANCE
C VALUES OVER A CERTAIN PORTION OF THE X-AXIS. FOR SPECIES
C WHICH HAVE HIGHLY STRUCTURED PEAKS, THIS MAY BE A VERY SHORT
C DISTANCE (E.G., METHANE USES A 2 CM-1 ONE ONE SIDE OF THE
C ANALYTICAL PEAK AND A 1.0 CM-1 INTERVAL ON THE OTHER. THESE
C INTERVALS ARE BASED ON EXPANDED PLOTS AND ARE CHOSEN TO GIVE
C POINTS CLOSE TO THOSE ONE WOULD CHOOSE IF DOING THE BASELINE
C CORRECTION BY HAND). THE SAME THING IS DONE ON THE OTHER
C SIDE OF THE ANALYTICAL PEAK. THESE POINTS WILL BE DEFINED
C WITHIN THE SUBROUTINE FOR EACH SEPARATE SPECIES.
C *****
C
C
C TO CONFORM WITH LOTUS 1-2-3 DATE FORMAT, READ THE VALUE OF
C RTP, THEN PRINT THIS AS LDATE
C
      LDATE = IRVAL(13751,0)

C TO AVOID EXTRA CHARACTERS IN THE TIME PRINTOUT,
C PICK OUT THE CHARACTERS NEEDED FROM THE IDATA ARRAY AND
C CONCATENATE THEM INTO THE NECESSARY OUTPUT.
C
      DO 25 I=58,65
        IF (I.EQ.58) THEN
          H1=CHAR(IDATA(I))
        ELSEIF (I.EQ.59) THEN
          H2=CHAR(IDATA(I))
        ELSEIF (I.EQ.61) THEN
          N1=CHAR(IDATA(I))
        ELSEIF (I.EQ.62) THEN
          N2=CHAR(IDATA(I))
        ELSEIF (I.EQ.64) THEN
          S1=CHAR(IDATA(I))
        ELSE (I.EQ.65)
          S2=CHAR(IDATA(I))
        ENDIF
25    CONTINUE
C
C CONCATENATE THE APPROPRIATE IDATA ELEMENTS TO FORM TIME
C CHARACTERS WHICH CAN BE PRINTED.
C
      HH = H1 // H2

```

```

      NN = N1 // N2
      SS = S1 // S2
C
C RETRIEVE THE TEMPERATURE CHARACTERS FROM THE IDATA ARRAY
C (THESE CHARACTERS ARE WRITTEN TO THE IDATA ARRAY DURING DATA
C ACQUISITION UNDER THE MACRO IR7 [SUB-MACRO AQ6] WITH THE
C FORTRAN PROGRAM "OTEMP.FTN")
C
      CT1=CHAR(IDATA(68))
      CT2=CHAR(IDATA(69))
      CT3=CHAR(IDATA(70))
      CT4=CHAR(IDATA(71))
C
C NOW, CONCATENATE THESE CHARACTERS TO FORM THE TEMPERATURE
C
      CTEMP=CT1 // CT2 // CT3 // CT4
C
C RETRIEVE THE RELATIVE HUMIDITY CHARACTERS FROM THE IDATA
C ARRAY (THESE CHARACTERS ARE WRITTEN TO THE IDATA ARRAY
C DURING DATA ACQUISITION UNDER THE MACRO IR7 [SUB-MACRO AQ6]
C WITH THE FORTRAN PROGRAM "RH.FTN")
C
      RH1=CHAR(IDATA(238))
      RH2=CHAR(IDATA(239))
      RH3=CHAR(IDATA(240))
      RH4=CHAR(IDATA(241))
      RH5=CHAR(IDATA(242))
      RH6=CHAR(IDATA(243))
C
C NOW, CONCATENATE THE %RH DATA INTO FINAL FORM
C
      HUMID= RH1 // RH2 // RH3 // RH4 // RH5 // RH6
C
C DETERMINE WHICH SPECIES ARE TO BE ANALYZED.
C
      844 IF (IFLAG1.EQ.1) CALL HZ(Y,FXAX,CABS)
           A1=CABS
C      IF (IFLAG2.EQ.1) CALL MMH(Y,FXAX,CABS)
           A2=CABS
C      IF (IFLAG3.EQ.1) CALL UDMH(Y,FXAX,CABS)
           A3=CABS
C      IF (IFLAG4.EQ.1) CALL CH4(Y,FXAX,CABS)
           A4=CABS
C      IF (IFLAG5.EQ.1) CALL SF6(Y,FXAX)
           A5=CABS
C      IF (IFLAG6.EQ.1) CALL NH3(Y,FXAX,CABS)
           A6=CABS
C
C PRINT OUT THE DATE, TIME, TEMPERATURE, ABSORBANCE
C VALUES, AND HUMIDITY

```



```

C
850 PRINT 150,LDATE,HH,NN,SS,CTEMP,A1,A4,A6,HUMID
150 FORMAT(' ',I5,2X,3(A2,2X),A4,2X,3(F6.3),2X,A6)
C
      GOTO 999
C
C FORMAT STATEMENTS USED BY ERROR DETECTION ROUTINES
C
900 WRITE(2,990) IDATA(10)
901 FORMAT(' ',/, ' ONLY DIMENSIONED TO ',I6,' PTS', ' NOT ',I6
1,/,)
902 FORMAT(' ', 'WHY ARE THERE ONLY ',I6,' PTS. REQUESTED?',/,)
990 FORMAT(' ',//, ' ABSORBANCE FLAG = ',I2,2X, 'NOT AN ABSORBAN
ICE FILE',//)
999 CONTINUE
      CALL EXIT
      END

```